National Aeronautics and
Space Administration

# HIGH-END COMPUTING CAPABILITY PORTFOLIO

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NASA Advanced Supercomputing Division

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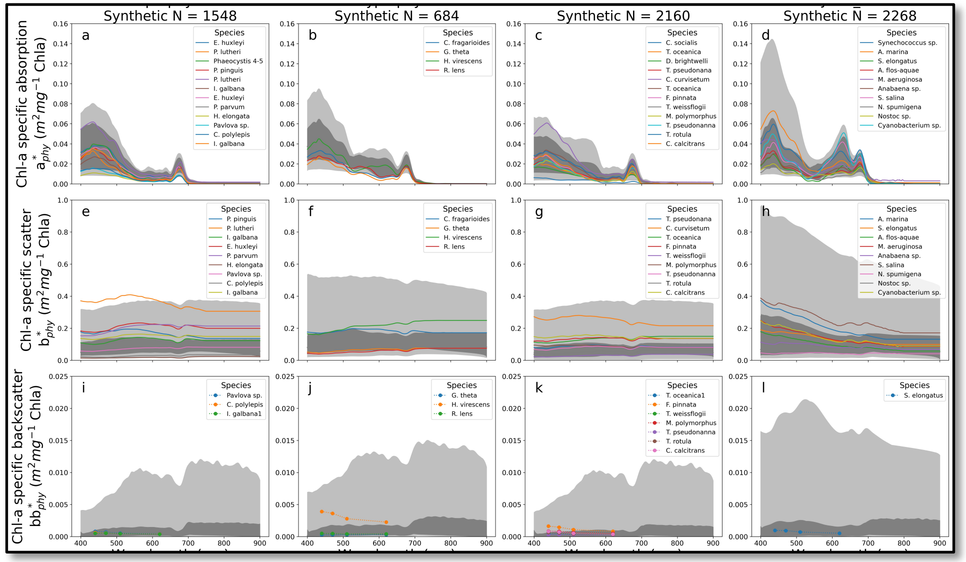
# Data Science Team Speeds up Data Generation for SWIPE Project

- The Data Science team used the Dask library to speed up the data-generation process for the Spectral Water Inversion Processor and Emulator (SWIPE) tool, which is used by the Biospheric Science team at NASA Ames to generate synthetic bio-optical datasets of alga particles for modeling water quality.
  - The Dask programing framework allows for the distribution of Python code across multiple CPUs and multiple nodes. Modules, such as dask.delayed, can be used to run python code in parallel.
- By embedding dask.delayed into SWIPE’s Equivalent Algal Populations component (EAP), the Data Science team reduced the time the SWIPE tool takes to create synthetic data and generate a spectral library for a single alga particle on one Broadwell node from 2 hours to 18.5 minutes.
  - EAP calculates the optical properties of water with alga and other phytoplankton species present—key in determining the degree of water contamination.
- The speedup will significantly reduce time-to-solution, as there are over 70 phytoplankton species that need to be modeled. A further reduction in solution time might be achieved by using Dask on multiple nodes.

IMPACT: Employing Dask supports the ultimate goal of the SWIPE project to build a neural network model that uses image data to determine the water quality of imaged water. The HECC effort increased the rate of spectral data generation by six times, speeding up synthetic data creation for NASA’s bio-optical modeling work.



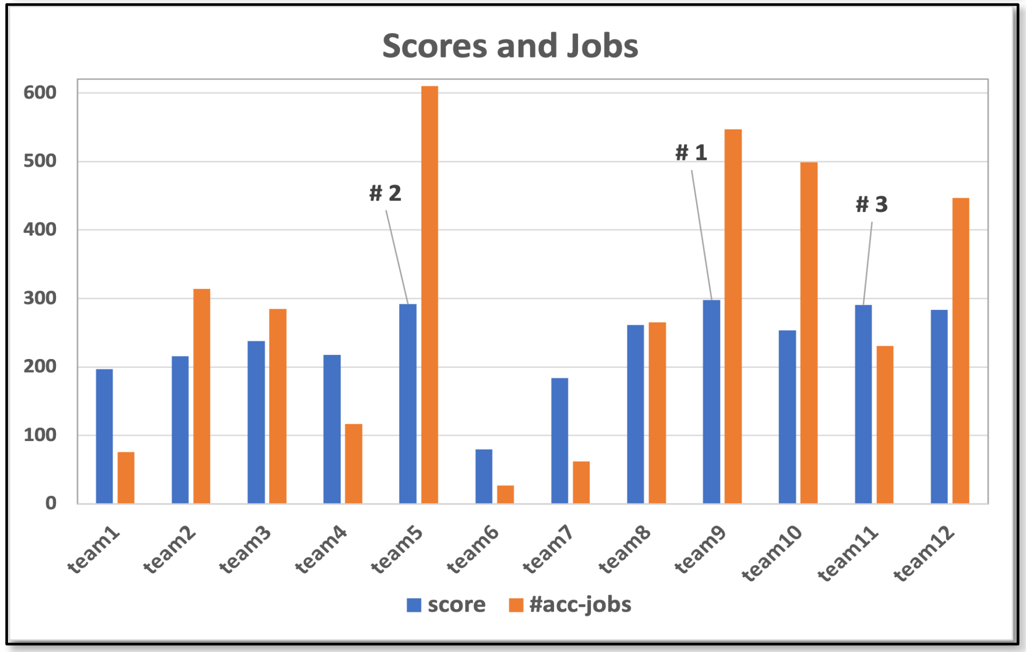

Synthetic spectral libraries of inherent optical properties: absorption (top row), total scatter (middle row), and backscatter (bottom row), for four groups of phytoplankton modeled for SWIPE.
*Jeremy Kravitz, NASA/Ames*

# HECC Mentors 2022 Winter Classic Invitational Student Cluster Competition

- HECC support staff represented NASA as one of four mentor HPC data centers (including Hewlett Packard Enterprise (HPE), Oak Ridge National Lab, and Amazon) to host the second student competition organized by Intersect360 Research. The competition provided hands-on experience with real HPC systems and applications for 12 teams from six Historically Black Colleges and Universities (HBCUs) and four Hispanic Serving Institutions (HSIs).
- The NASA segment of the competition took place from March 6 – 12. In total, 32 of the 48 students from the 12 teams submitted 3,480 batch jobs to run on 52 Pleiades Sandy Bridge nodes, consuming 3,991 standard billing units (SBUs*).
- HECC User Services staff worked with the 48 students to complete account applications in time for the competition and assisted them with onboarding.
- The Application Performance and Productivity team selected the Multi-Zone version of the NAS Parallel Benchmarks (NPB-MZ) for the competition, prepared an online training video and slides and two live Q & A sessions, and mentored the students on running and optimizing the selected benchmarks via Slack channels.
- The NASA Module Results were announced publicly by Intersect360: https://www.winterclassicinvitational.com/winter-classic-2022-nasa-results-in/
- This event proved to be rewarding, as one student stated: “Thank you NASA mentors for the training and allowing us to use and learn on your systems. I have really enjoyed working with you and learning more about HPC.”

**1 SBU equals 1 hour of a Pleiades Broadwell 28-core node.*

**IMPACT**: The cluster competition gives NASA an opportunity to attract new talent and empowers HBCU and HSI students with skills that will prepare them for positions in high performance computing.

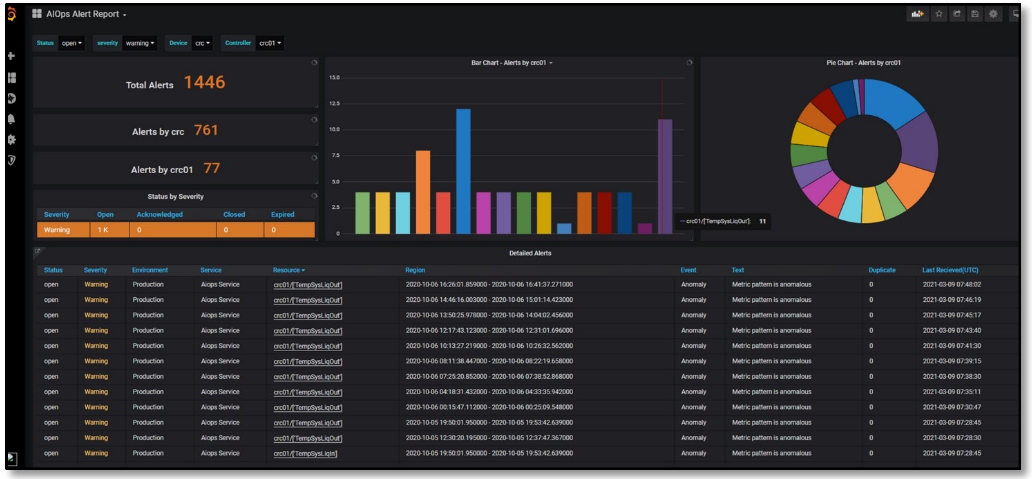



Correlation between number of jobs submitted and the final score (sum of normalized score from the three benchmarks) achieved by each team. The top teams tended to put in more efforts by submitting many jobs which explored various optimization spaces. *Henry Jin, NASA/Ames*

# Aitken Rome HPCM Upgrade Improves System Monitoring

- The HECC Systems team upgraded the HPE Performance Cluster Manager (HPCM) from version 1.4 to 1.6. HPCM is HPE's provisioning software solution for HPC clusters used on the Aitken Rome nodes.
- The upgrade was driven by NASA security requirements and take into account:
  - SUSE Linux Enterprise Server (SLES) 15 SP2 reached the end of its lifecycle in January 2022;
  - HPCM 1.4 is not supported on SLES 15 SP3;
  - HPCM 1.6 is the latest version supported on SLES 15 SP3.
- Systems staff also improved the reliability of the HPCM 1.6 console via several code fixes.
- Additional custom changes to HPCM 1.6 include:
  - Added support for multiple hostnames and node aliases
  - Enabled adding new/changing existing options to the Named daemon.
  - Added Dynamic Host Configuration Protocol (DHCP) options for maximum/default lease times.
  - Enabled per-line timestamps to console logs.
  - Improved performance of su-leader-setup to support a future process.

**IMPACT**: Upgrading to HPCM 1.6 solves several issues, including fixing a compute node console connectivity issue and improving access to HECC console logs, which enhances system engineers' ability to troubleshoot user job failures.




Screenshot of the HPE Performance Cluster Manager (HPCM) dashboard. *Image courtesy of HPE.*

# Merope Supercomputer Ends Eight Years of Service

- After eight years of number crunching, the Merope supercomputer was decommissioned on March 25, 2022. The system was used for running both real-world computational jobs for NASA scientists and engineers and for testing purposes. While the system became unavailable to users in May 2021, it continued to be used for InfiniBand testing by system administrators until this month.
- Merope, which became operational in September 2013, was originally comprised of Intel Xeon X5670 (Westmere) and Intel Xeon 5400 (Harpertown) processors repurposed from Pleiades nodes to accommodate jobs that ran more efficiently on older hardware.
- The final version of Merope comprised 56 racks, 1,792 nodes, and 21,504 total Westmere cores, with 86 terabytes total memory and 256 teraflops theoretical peak performance.
- The decision to decommission Merope was based on a cost analysis.
  - Ongoing expenses to run the 21,000 cores were significantly higher compared to newer architectures.
  - In terms of standard billing units (SBUs*), the system was comparable to one rack of AMD Rome nodes.
  - Electrical and cooling was eight times more expensive to run compared to equivalent Rome nodes.
  - Node failure rate was high, preventing productive use of the aging system.

**1 SBU equals 1 hour of a Pleiades Broadwell 28-core node.*

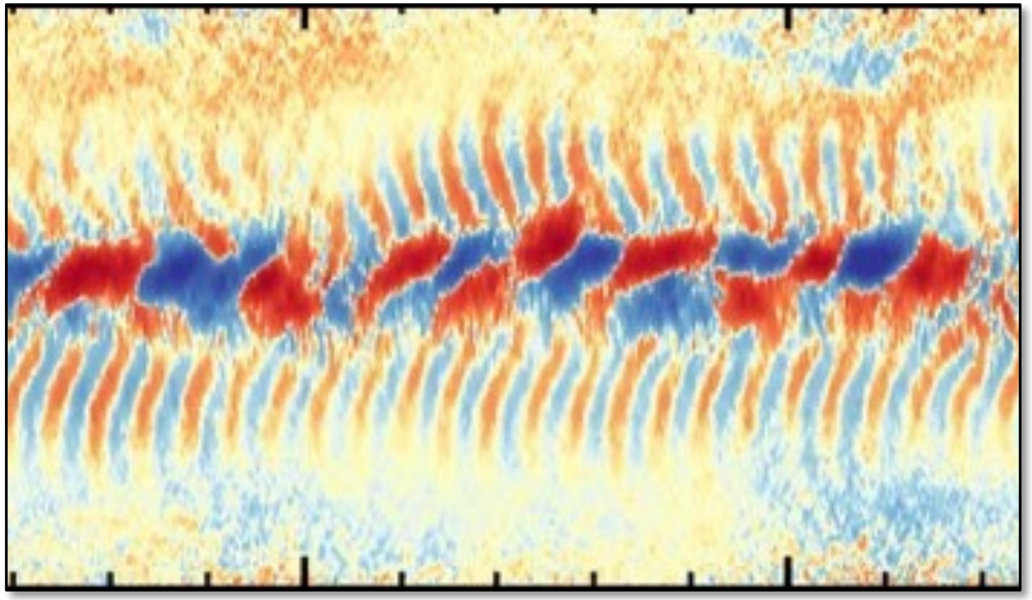
**IMPACT**: The cost savings associated with decommissioning this aging system—approximately $600 thousand per year—allows the HECC project to purchase newer architectures and provide more resources to the NASA user community.


Merope racks on the data center floor in Building N233A at NASA's Ames Research Center. *Chris Tanner, NASA/Ames*

# Simulating the Many Personalities of Our Sun*

- Researchers at the University of Colorado Boulder ran 3D magnetic fluid simulations on Pleiades that capture several cyclical features of solar magnetism and the propagation of magnetic flux toward the poles. The simulations suggest that the Sun may be a chaotic dynamical system residing in a state of bistability—a bifurcation regime in which two distinct dynamos can operate simultaneously or in tandem.
- The simulations achieved remarkable dynamo behaviors similar to observed features of the solar cycle:
  - A highly regular cycling system in which four “magnetic wreaths”—tubes of magnetic flux that wrap all the way around a magnetized spherical shell in a large torus—steadily migrate toward the solar equator and regularly reverse their polarity, similar to the butterfly pattern found in the 11-year sunspot cycle.
  - The poloidal magnetic field eventually bifurcates: the system of four wreaths persists and cycles, but a new system of partial wreaths, each of opposite polarity, coexists superimposed on the original system.
- The simulations ran for weeks at a time and used up to 4,000 processors on Pleiades, producing terabytes of data that are stored on HECC systems.

**IMPACT**: These simulations provide major insights into how the solar dynamo operates and show that our Sun potentially exists in a “bistable” state, where these structures cycle superimposed on one another.



Extended time-latitude diagram of the simulated Sun’s azimuthal magnetic field at mid-convection zone. Panels show the longitude-averaged field as a function of time and latitude, with color intensity corresponding to field magnitude. Time is measured from the introduction of the magnetic field to the hydrodynamic progenitor. *Loren Matilsky, Juri Toomre, JILA / University of Colorado Boulder*

** HECC provided supercomputing resources and services in support of this work.*

# CFD Analysis of Mars Retrorocket Wind Tunnel Models*

- Supersonic retropropulsion (SRP) technology offers an alternative to large parachutes for decelerating a spacecraft during atmospheric descent at Mars. Researchers at NASA Langley Research Center (LaRC) developed a computational fluid dynamics (CFD) model to analyze a range of supersonic descent conditions to support planned observational tests in the Langley Unitary Plan Wind Tunnel (UPWT) in 2022.
- The Langley team conducted CFD analysis on a range of wind tunnel conditions and model configurations, including three tunnel Mach numbers, three model thrust levels and attitudes, and six different nozzle designs.
- Information generated during the CFD and testing process will be used to:
  - Establish CFD best practices for modeling SRP flow fields
  - Inform the planning of future SRP wind tunnel tests with improved testing and measurement methods
  - Compare the total required resources required to execute the wind tunnel test and the CFD simulations
  - Form the basis for uncertainty estimation of CFD methods at Mars SRP flight conditions
- Langley CFD analysts used over 30 million processor-hours to complete over 300 solutions on the Aitken, Electra, and Pleiades supercomputers. Each solution typically required computational meshes with tens to hundreds of millions of grid points and thousands of processor-hours on unsteady fluid dynamics problems.

** HECC provided supercomputing resources and services in support of this work.*

**IMPACT**: Most of these simulations could only be executed on HECC resources due to their large memory requirements. Comparisons between the CFD results and test data will form the basis for understanding how accurately and efficiently CFD methods can predict future Mars SRP vehicle performance.

Visualization of wind tunnel model air particles seeded at the nozzle entrances. *Bil Kleb, NASA/Langley; Timothy Sandstrom, NASA/Ames*

# Papers

- "**Separating Energetic Internal Gravity Waves and Small-Scale Frontal Dynamics**," H. Torres, et al., Geophysical Research Letters, vol. 49, issue 6, March 1, 2022. *
  *https://agupubs.onlinelibrary.wiley.com/doi/full/10.1029/2021GL096249*
- "**Multi-Fidelity Approach to Predicting Multi-Rotor Aerodynamics Interactions**," O. Pinti, et al., AIAA Journal, published online March 2, 2022. *
  *https://arc.aiaa.org/doi/full/10.2514/1.J060227*
- "**TOI-1696: A Nearby M4 Dwarf with a 3$R_{\oplus}$ Planet in the Neptunian Desert**," M. Mori, et al., arXiv:2203.02694 [astro-ph.EP], March 5, 2022. *
  *https://arxiv.org/abs/2203.02694*
- "**Direct Statistical Simulation of the Busse Annulus**," J. Oishi, et al., arXiv:2203.03699 [physics.flu-dyn], March 7, 2022. *
  *https://arxiv.org/abs/2203.03699*
- "**Non-Ideal Fields Solve the Injection Problem in Relativistic Reconnection**," L. Sironi, arXiv:2203.04342 [astro-ph.HE], March 8, 2022. *
  *https://arxiv.org/abs/2203.04342*
- "**TOI-1670 b and c: An Inner Sub-Neptune with an Outer Warm Jupiter Unlikely to have Originated from High-Eccentricity Migration**," Q. Tran, et al., arXiv:2203.04334 [astro-ph.EP], March 8, 2022. *
  *https://arxiv.org/abs/2203.04334*

** HECC provided supercomputing resources and services in support of this work*

# Papers (cont.)

- "**A Dynamo Simulation Generating Saturn-like Small Magnetic Dipole Tilts**," R. Yadav, H. Cao, J. Bloxham, Geophysical Research Letters, vol. 49, issue 5, March 9, 2022. *
*https://agupubs.onlinelibrary.wiley.com/doi/full/10.1029/2021GL097280*
- "**Computation of Hypersonic Viscous Flows with the Thermally Perfect Gas Model using a Discontinuous Galerkin Method**," E. Ching, et al., International Journal for Numerical Methods in Fluids, published online March 10, 2022. *
*https://onlinelibrary.wiley.com/doi/abs/10.1002/fld.5079*
- "**The Young HD 73583 (TOI-560) Planetary System: Two 10-$M_\oplus$ Mini-Neptunes Transiting a 500-Myr-Old, Bright, and Active K Dwarf**," O. Barragan, et al., Monthly Notices of the Royal Astronomical Society, Published online March 10, 2022. *
*https://academic.oup.com/mnras/advance-article/doi/10.1093/mnras/stac638/6548902*
- "**OJXPerf: Featherlight Object Replica Detection for Java Programs**," B. Li, et al., arXiv:2203.12712 [cs.PL], March 23, 2022. *
*https://arxiv.org/abs/2203.12712*
- "**AWSoM Magnetohydrodynamic Simulation of a Solar Active Region with Realistic Spectral Synthesis**," T. Shi, et al., The Astrophysical Journal, vol. 928, no. 1, March 24, 2022. *
*https://iopscience.iop.org/article/10.3847/1538-4357/ac52ab/meta*

** HECC provided supercomputing resources and services in support of this work*

# Papers (cont.)

- "**Schwarzchild and Ledoux are Equivalent on Evolutionary Timescales**," E. Anders, The Astrophysical Journal Letters, vol. 928, no. 1, March 25, 2022. *
*https://iopscience.iop.org/article/10.3847/2041-8213/ac5cb5/meta*
- "**Effects of Problem Complexity Reduction on Parameter Sensitivity and Classification in Charring Ablator Scenarios**," P. Rostkowski, et al., Aerospace Science and Technology, published online March 30, 2022. *
*https://www.sciencedirect.com/science/article/abs/pii/S1270963822001961*
- "**An Active Flow Control Approach for Spatially Growing Mixing Layer**," U. Kaul, Journal of Fluids Engineering, March 30, 2022. *
*https://asmedigitalcollection.asme.org/fluidsengineering/article-abstract/144/6/061110/1137820/An-Active-Flow-Control-Approach-for-Spatially*

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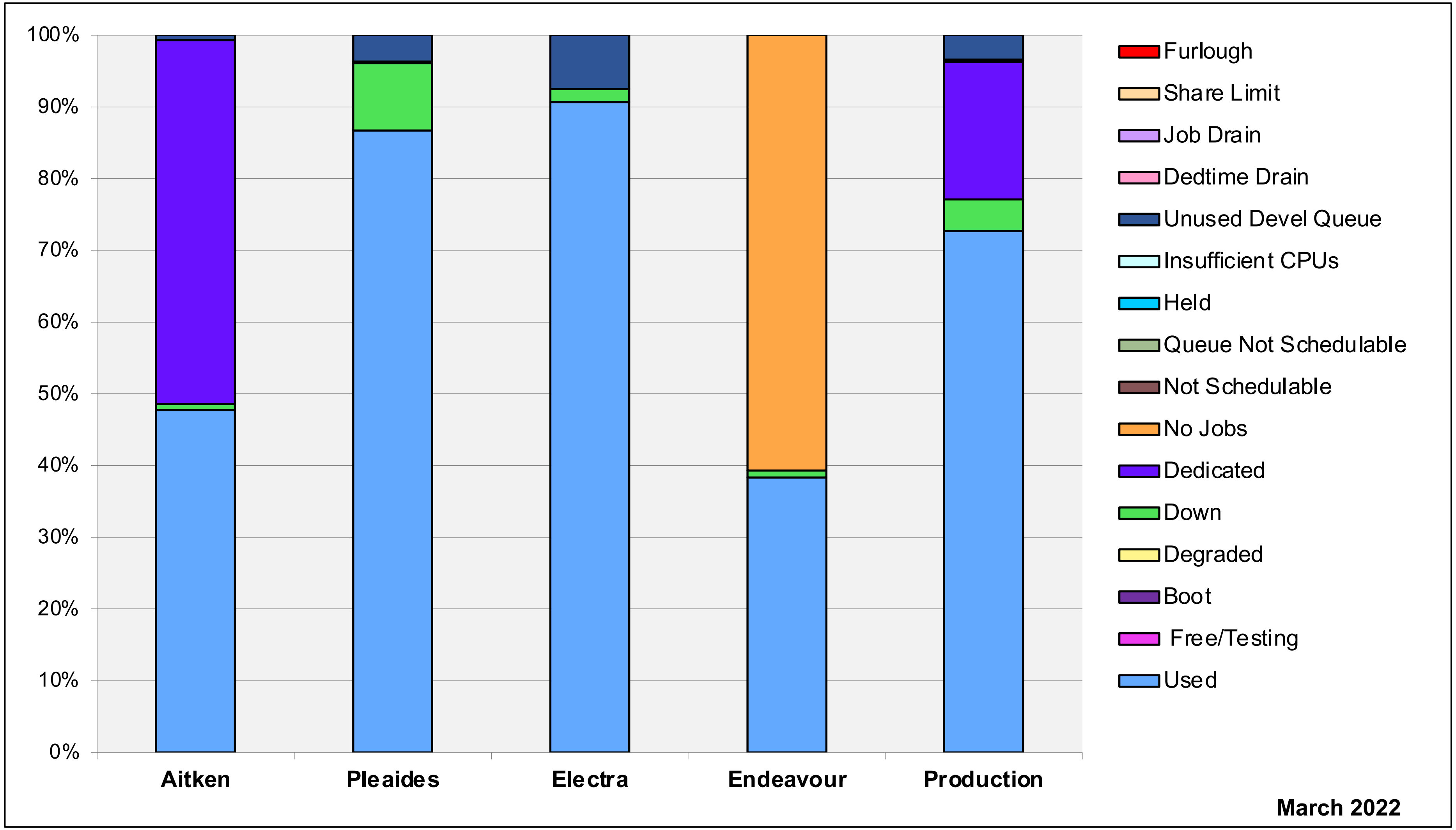
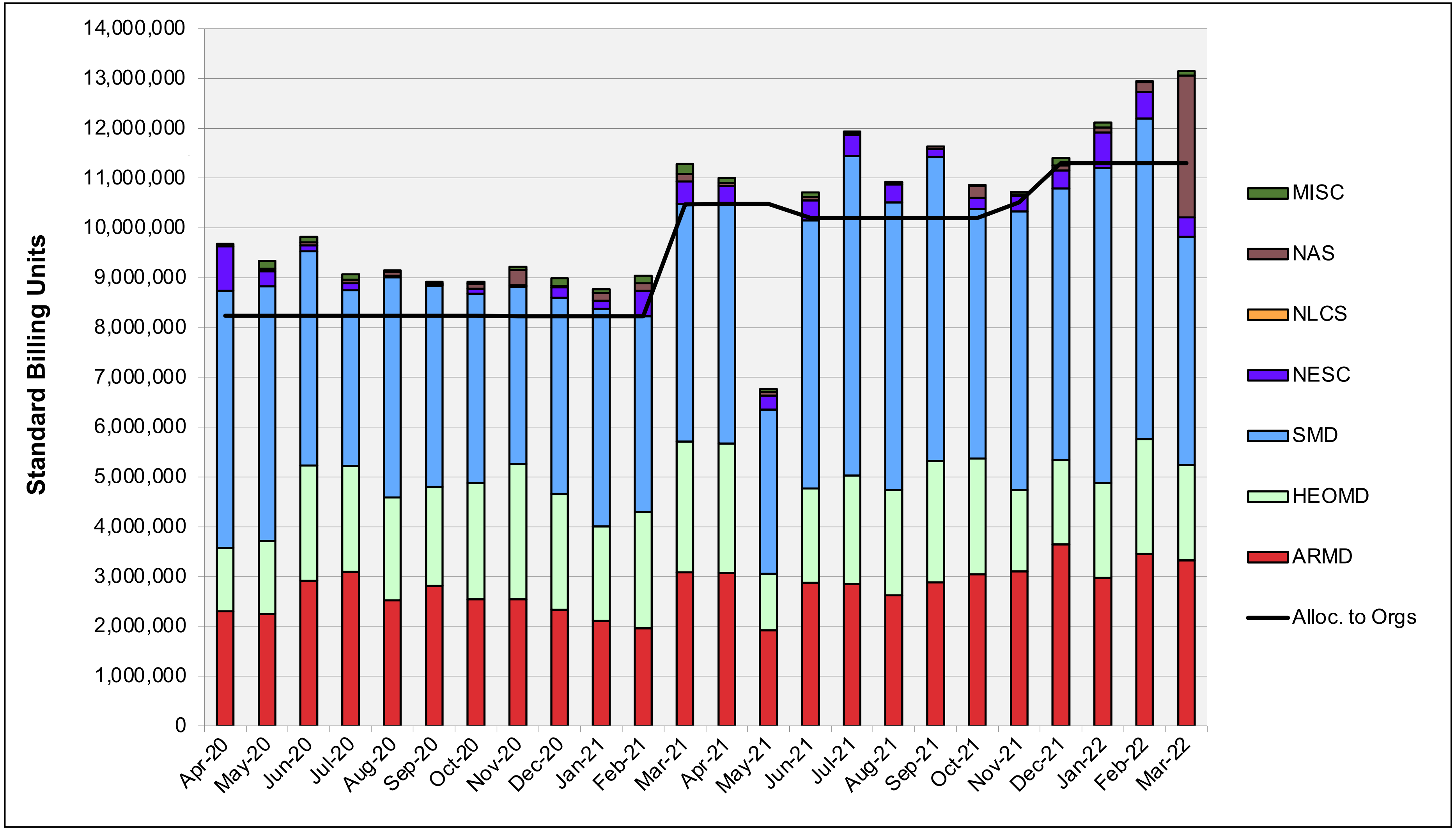
# News and Events

- **Ames' Contributions to the X-59 Quiet Supersonic Technology Aircraft**, *NASA Ames Feature*, March 21, 2022—NASA's Ames Research Center has decades of experience researching supersonic flight, much of which has gone into the unique design of the X-59. As Lockheed Martin Skunk Works finalized the X-59 airplane's design, they ran their ideas on the supercomputers at the NASA Advanced Supercomputing (NAS) facility using the Cart3D and LAVA simulation tools—both developed in the NAS Division.
  *https://www.nasa.gov/feature/ames/x-59*
  - **Ames' Contributions to the X-59 Quiet Supersonic Technology Aircraft**, *Military Aerospace*, March 25, 2022. *https://www.militaryaerospace.com/commercial-aerospace/article/14269974/ames-contributions-to-the-x59-quiet-supersonic-technology-aircraft*

# HECC Utilization



# HECC Utilization Normalized to 30-Day Month



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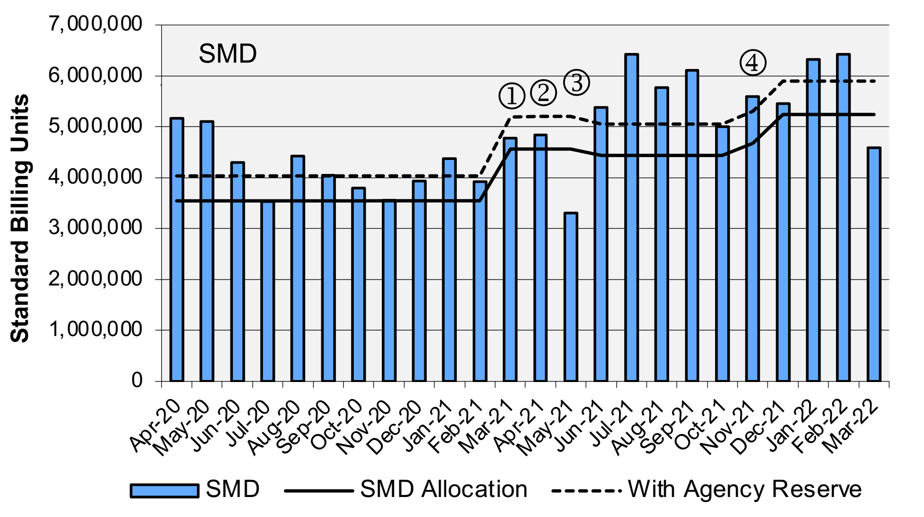
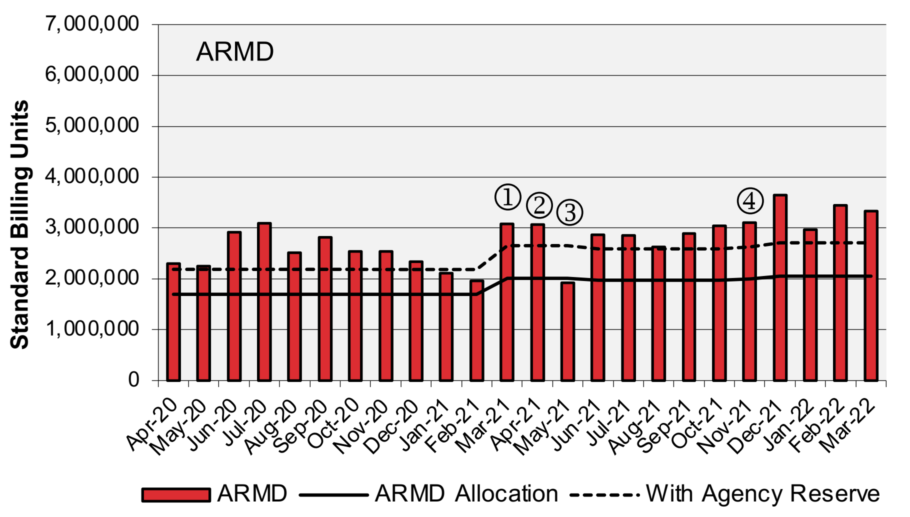
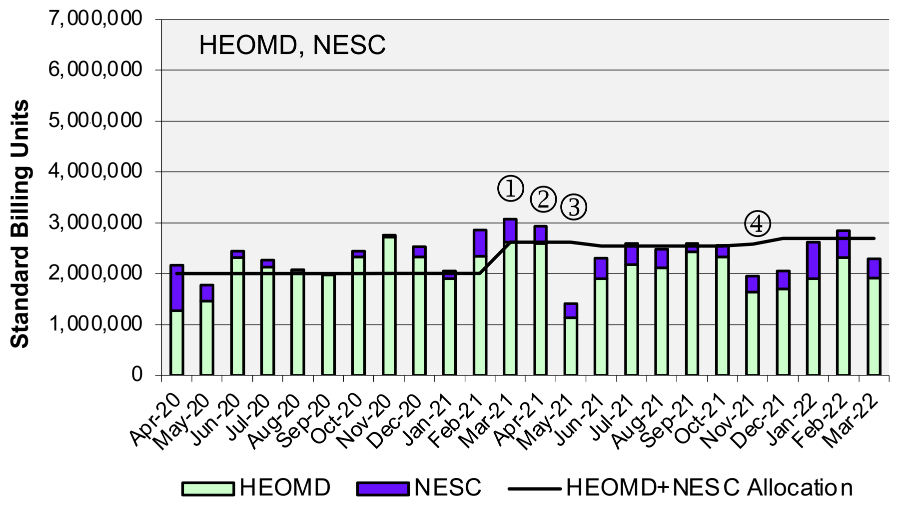


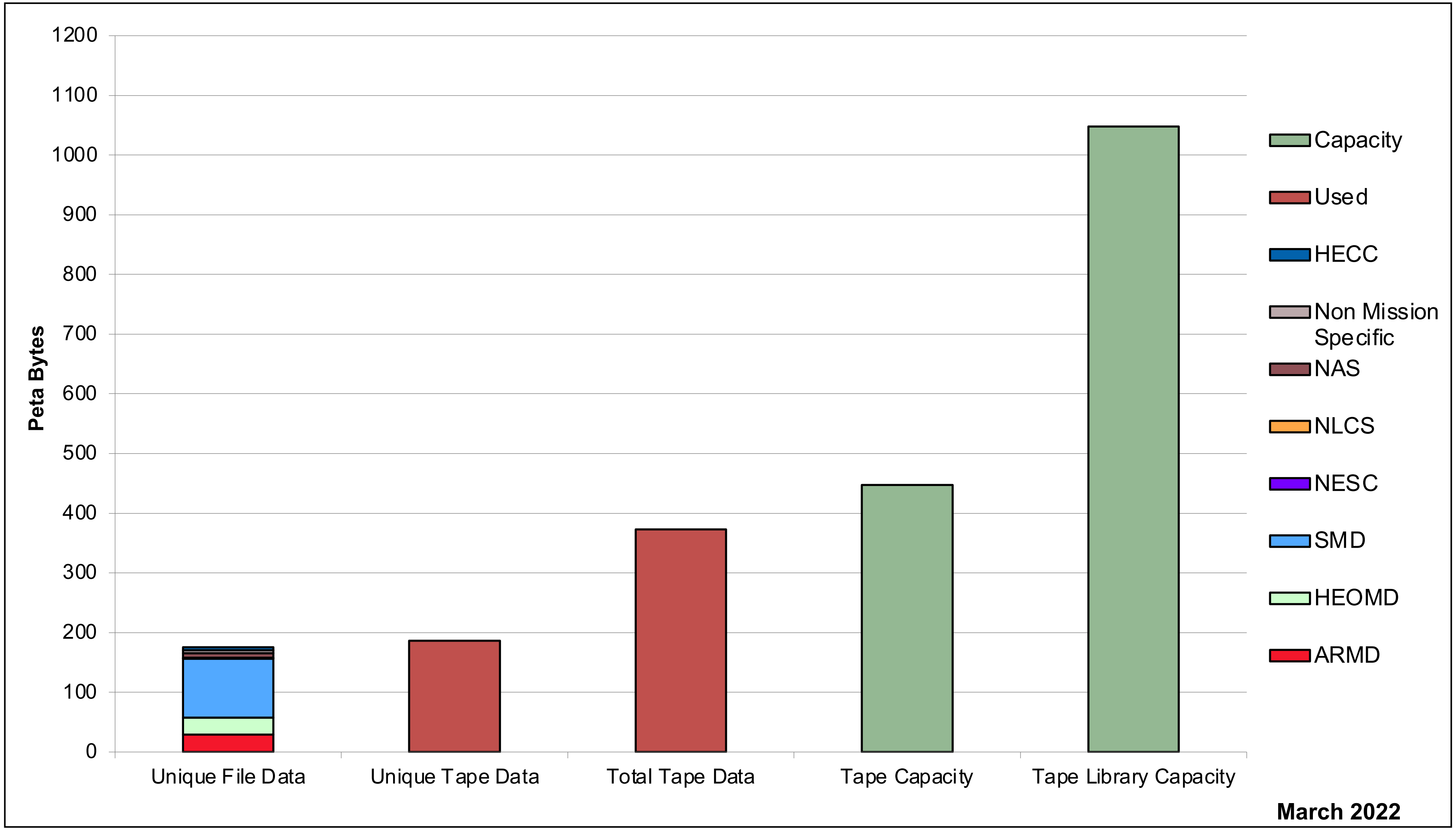

① 8 Rome Apollo racks introduced into Aitken

② Endeavour replaced with new hardware

③ Merope retired

④ 4 Rome Apollo Racks added to Aitken

# Tape Archive Status



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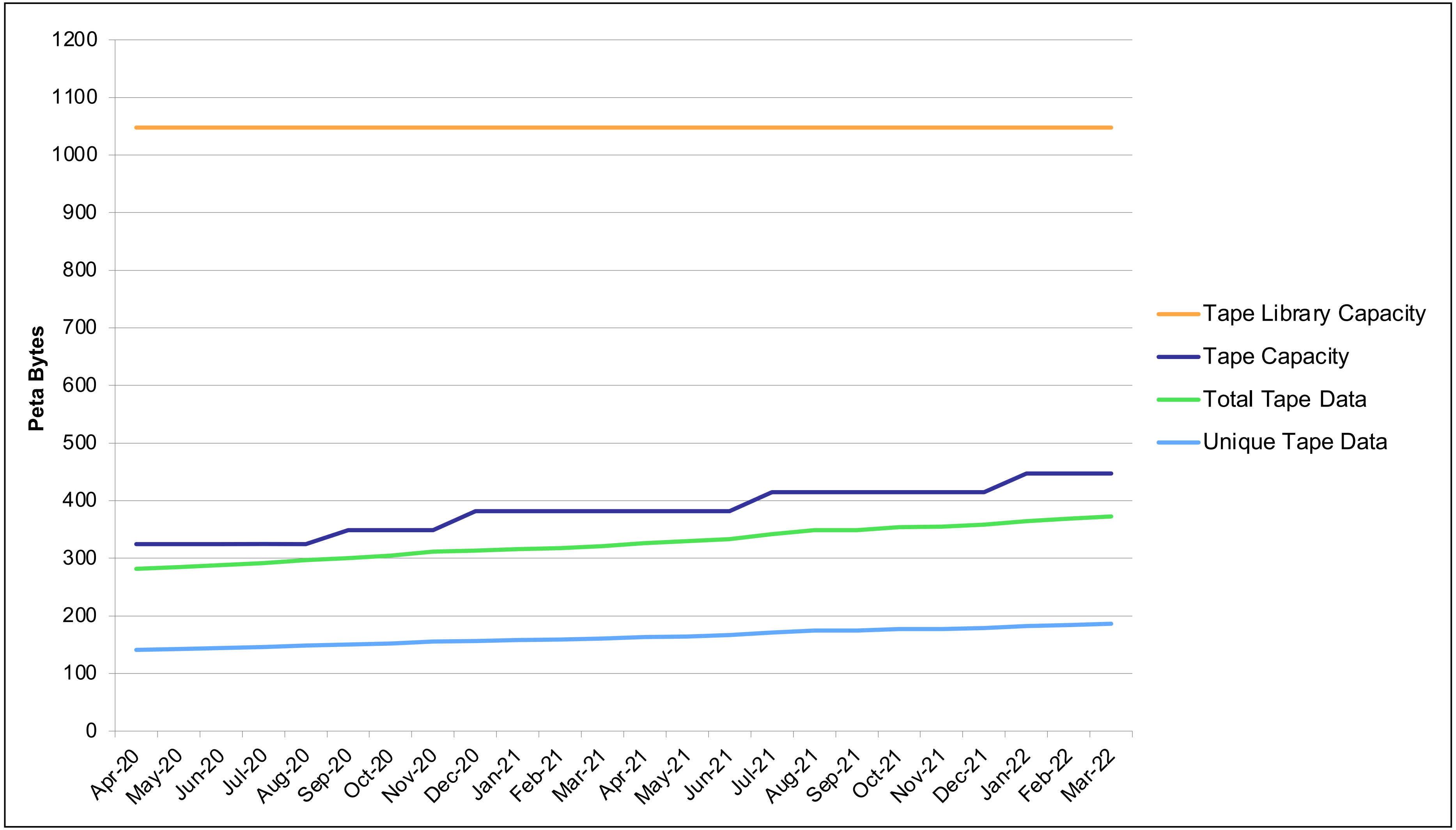
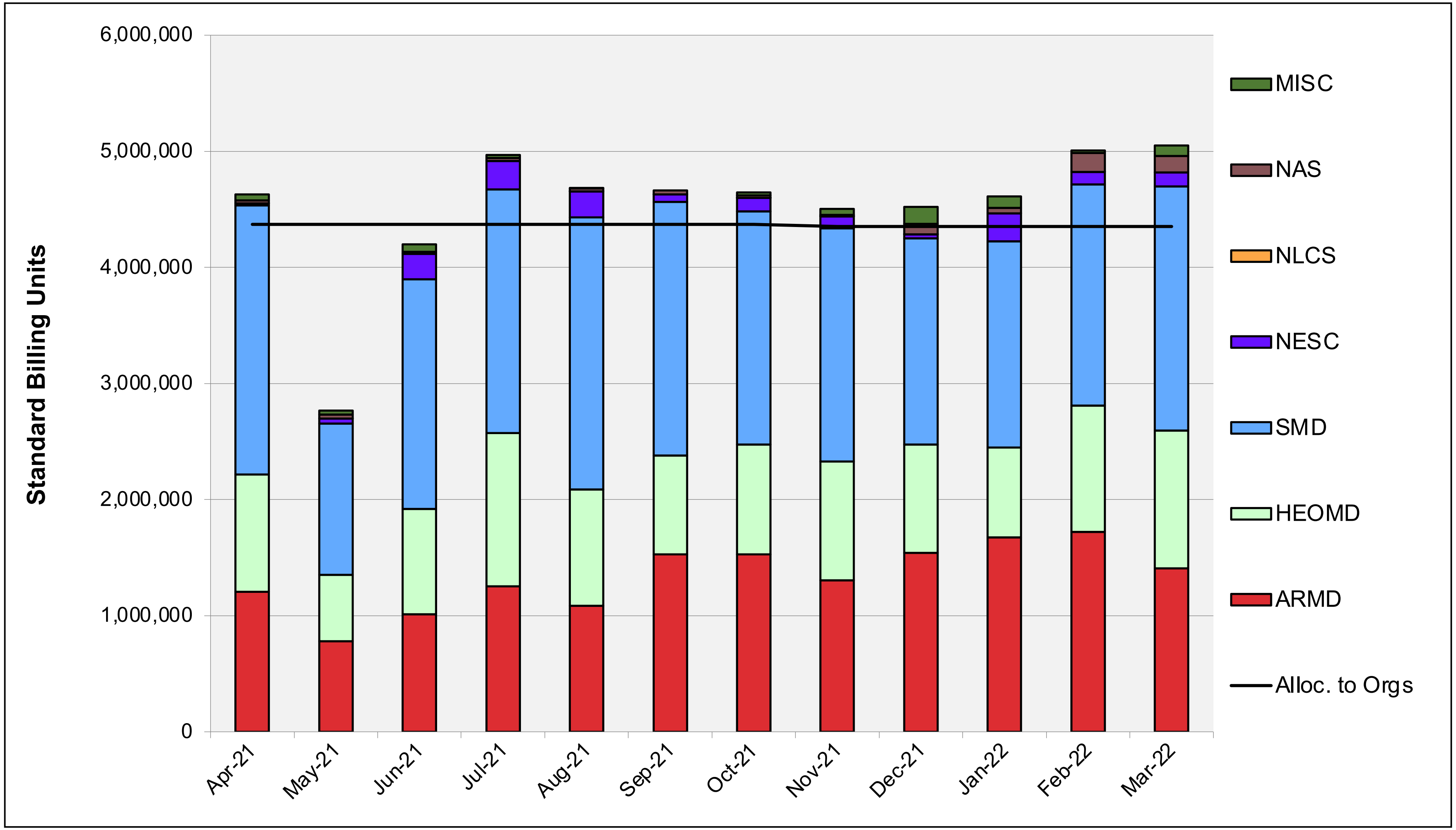
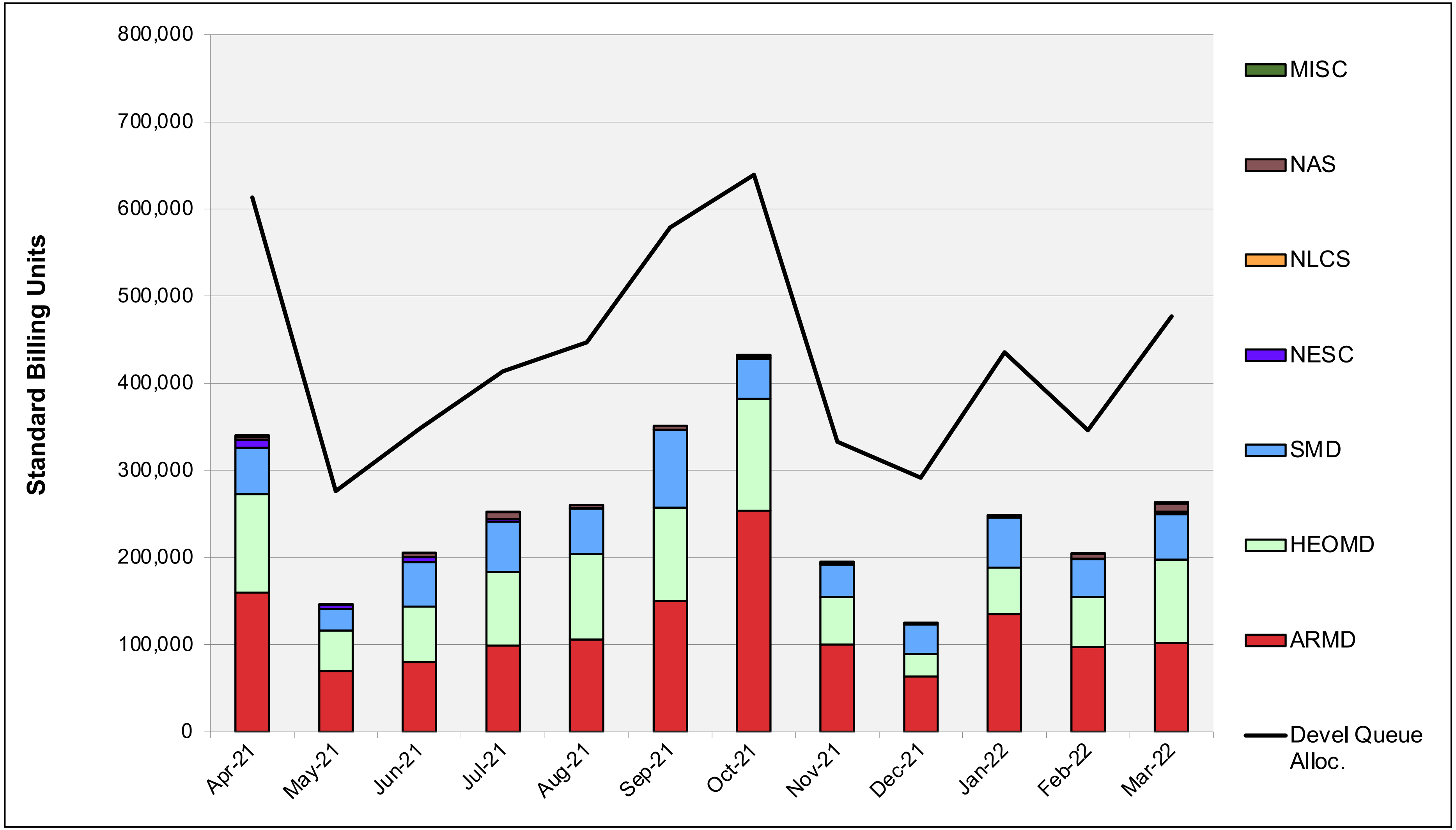


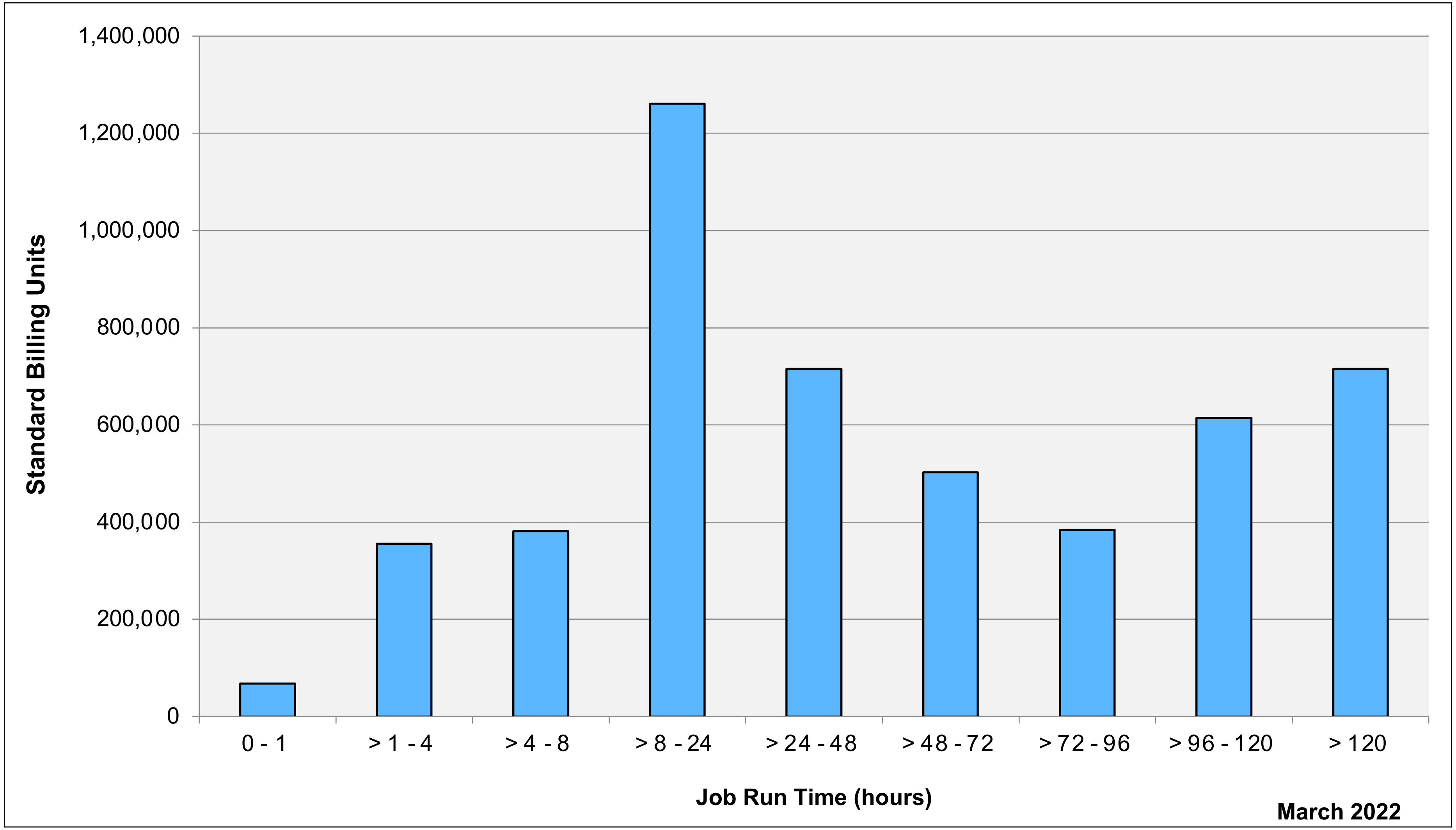
# Pleiades: SBUs Reported, Normalized to 30-Day Month



# Pleiades: Devel Queue Utilization



# Pleiades: Monthly Utilization by Job Length



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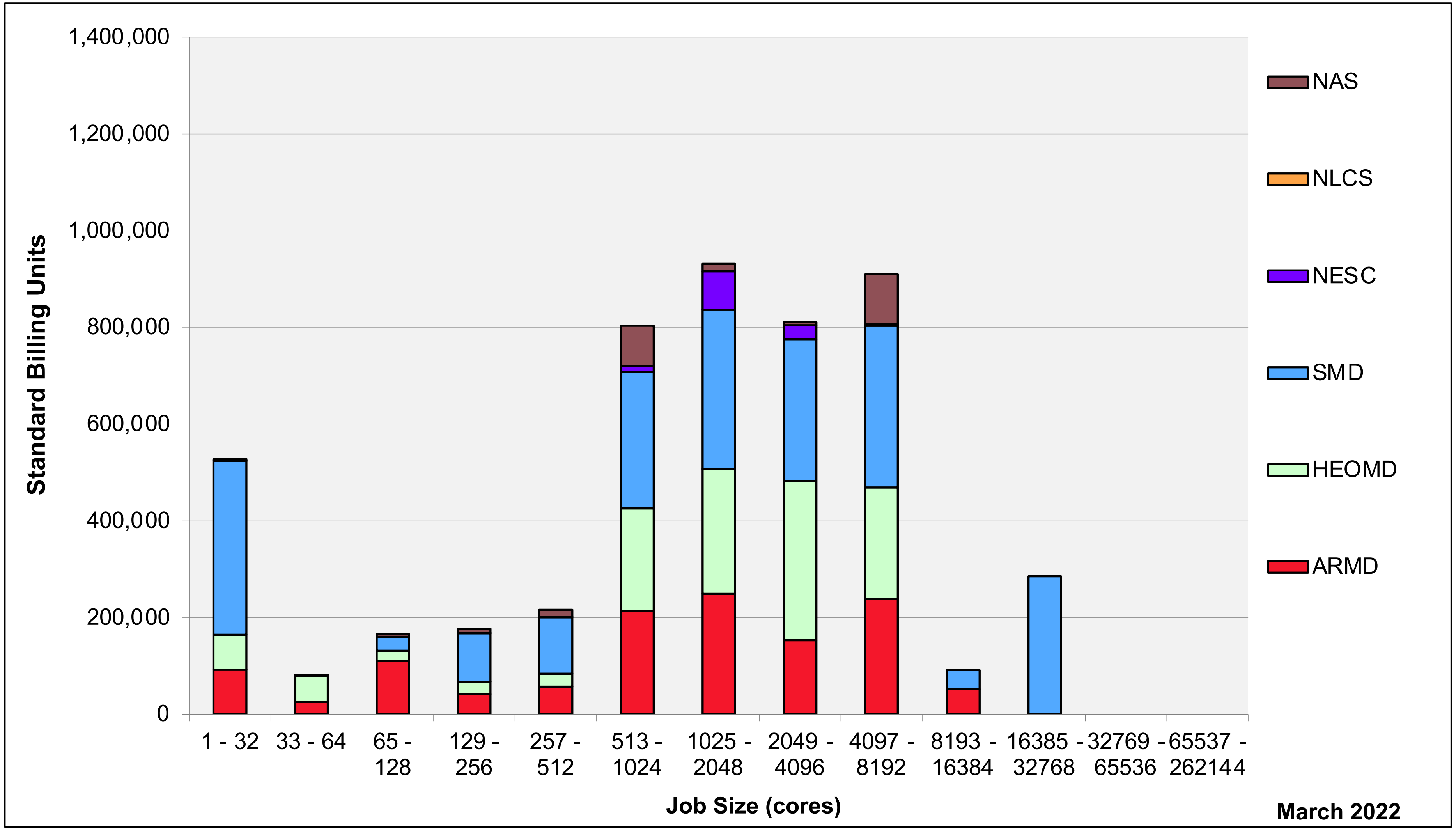

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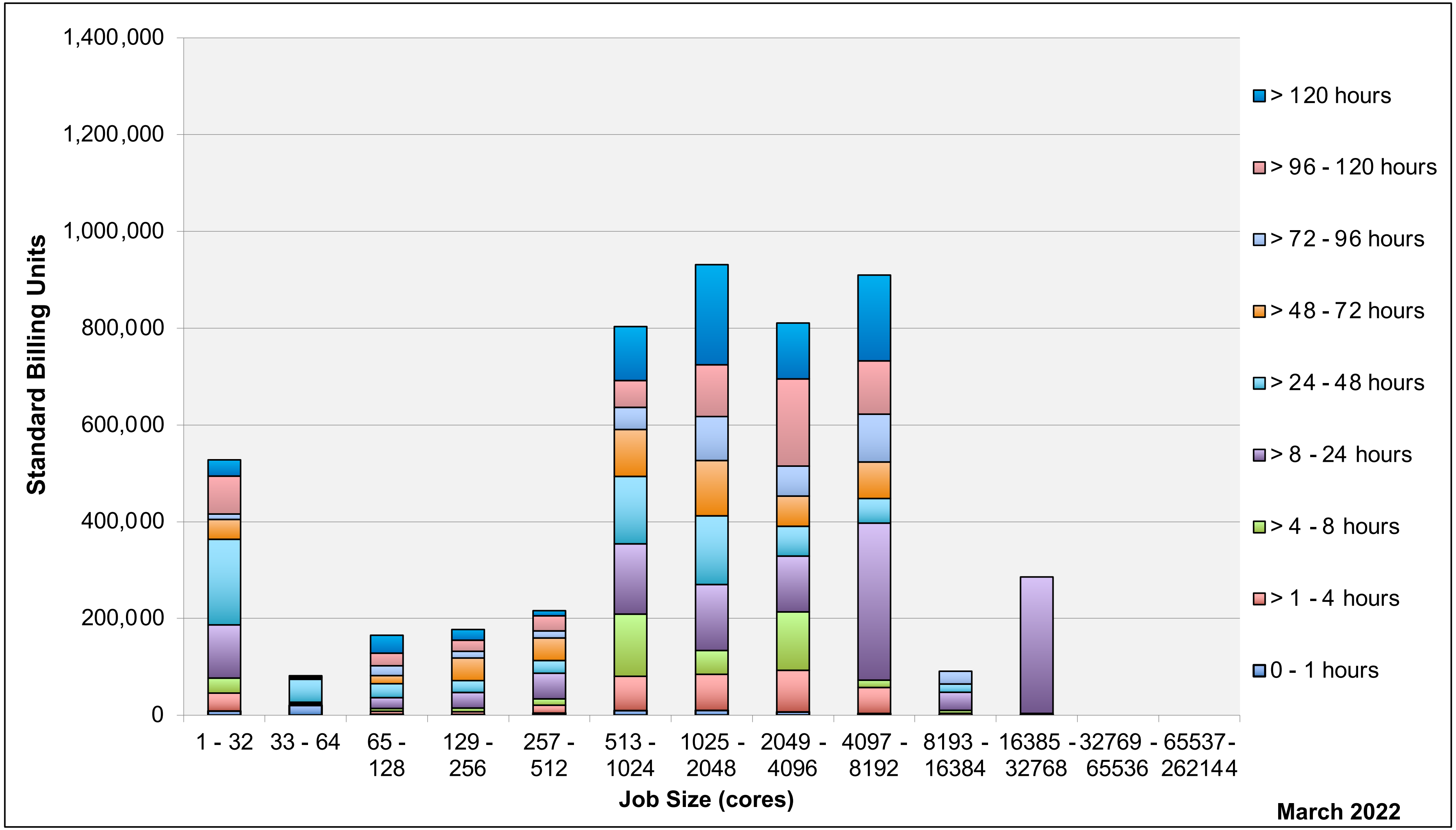
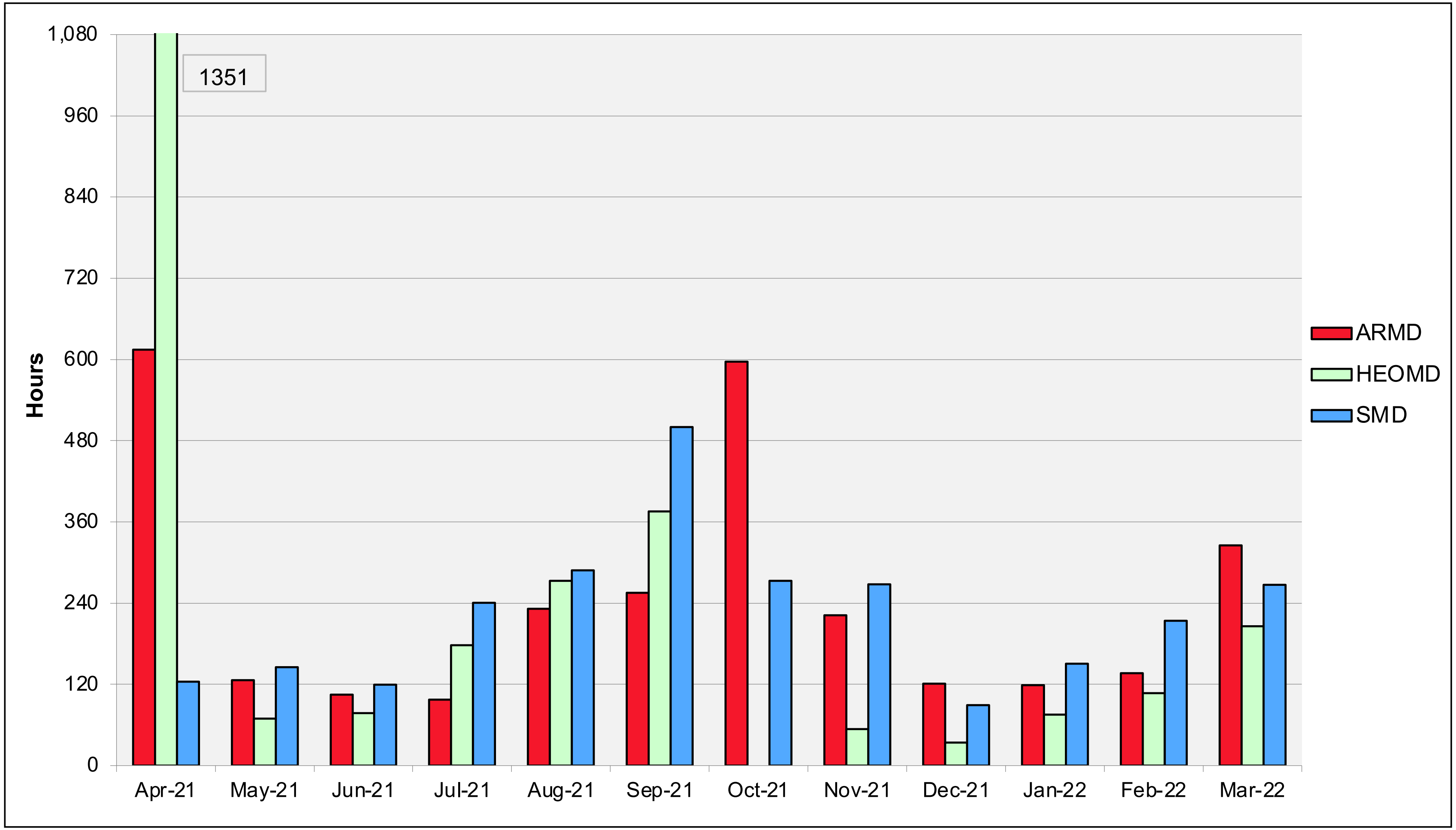
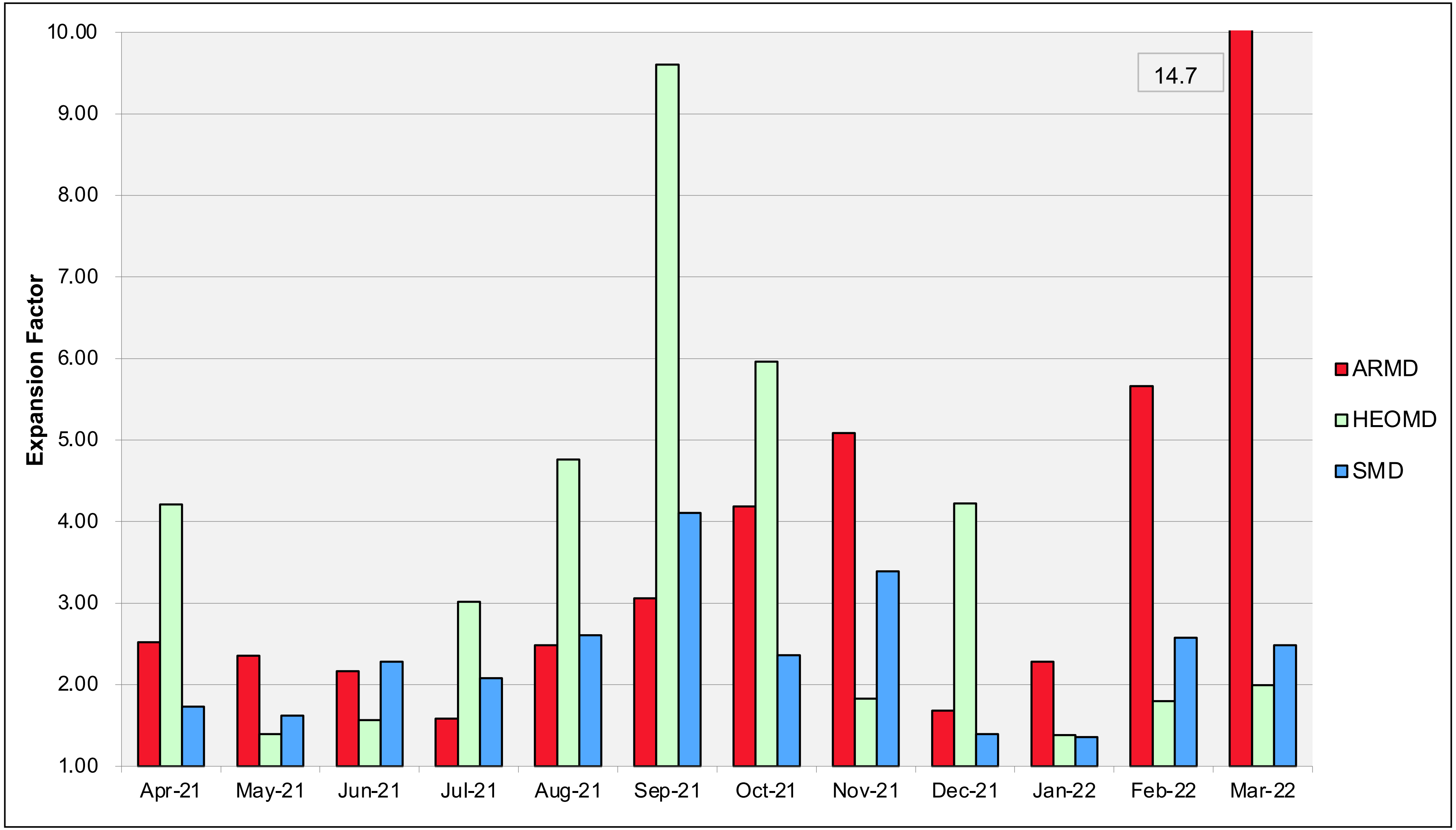


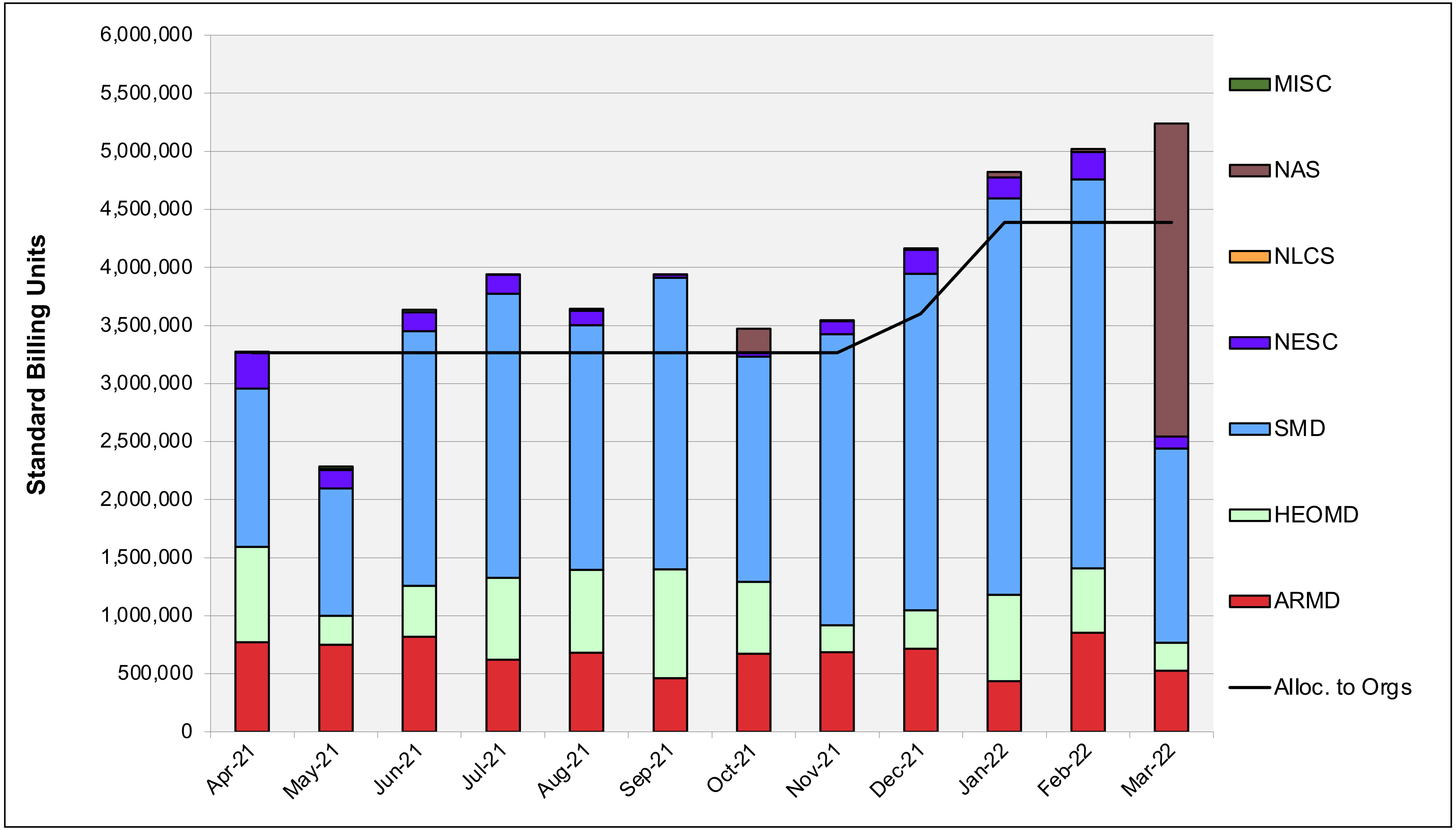
# Pleiades: Average Time to Clear All Jobs



# Pleiades: Average Expansion Factor



# Aitken: SBUs Reported, Normalized to 30-Day Month



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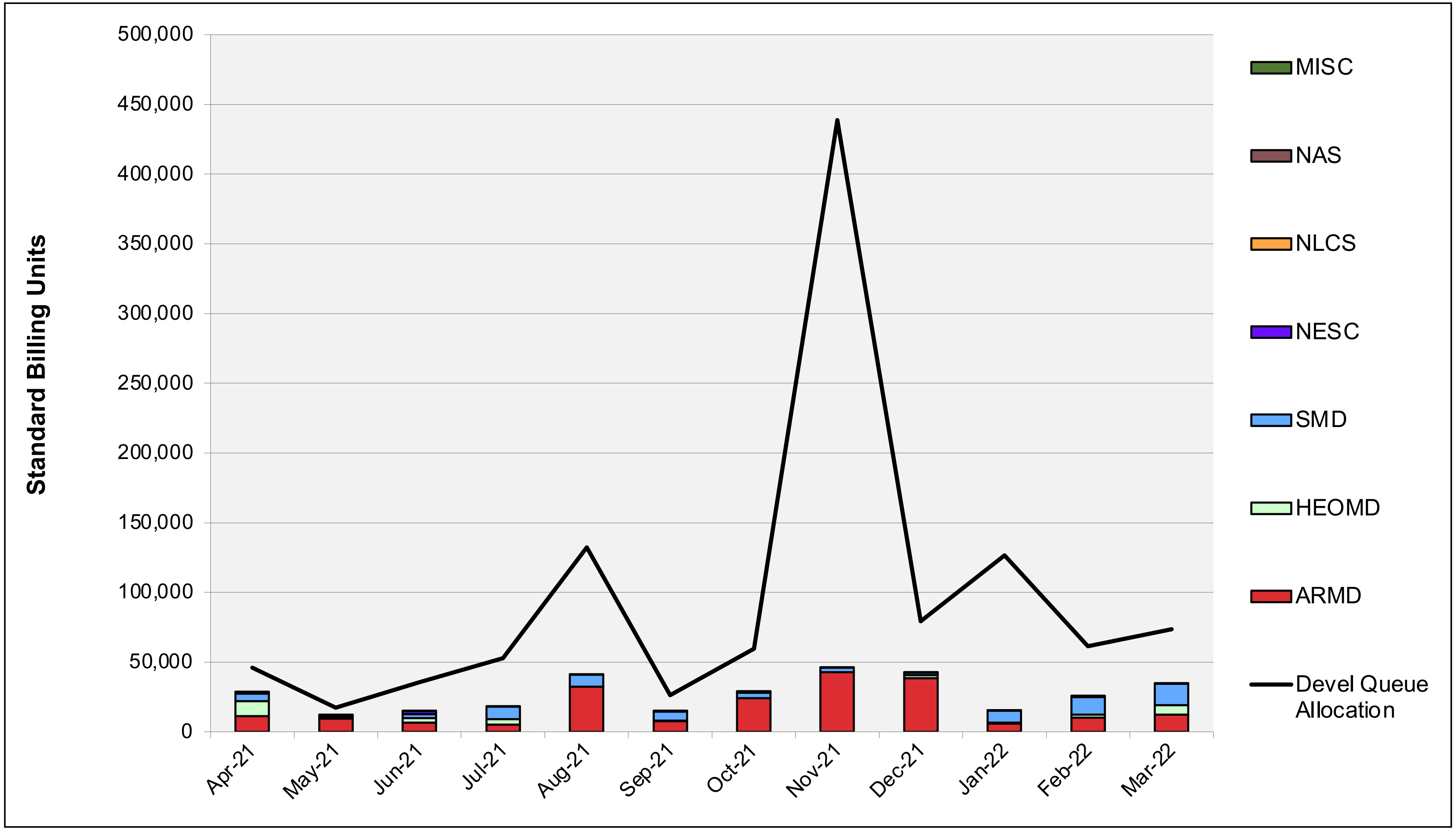

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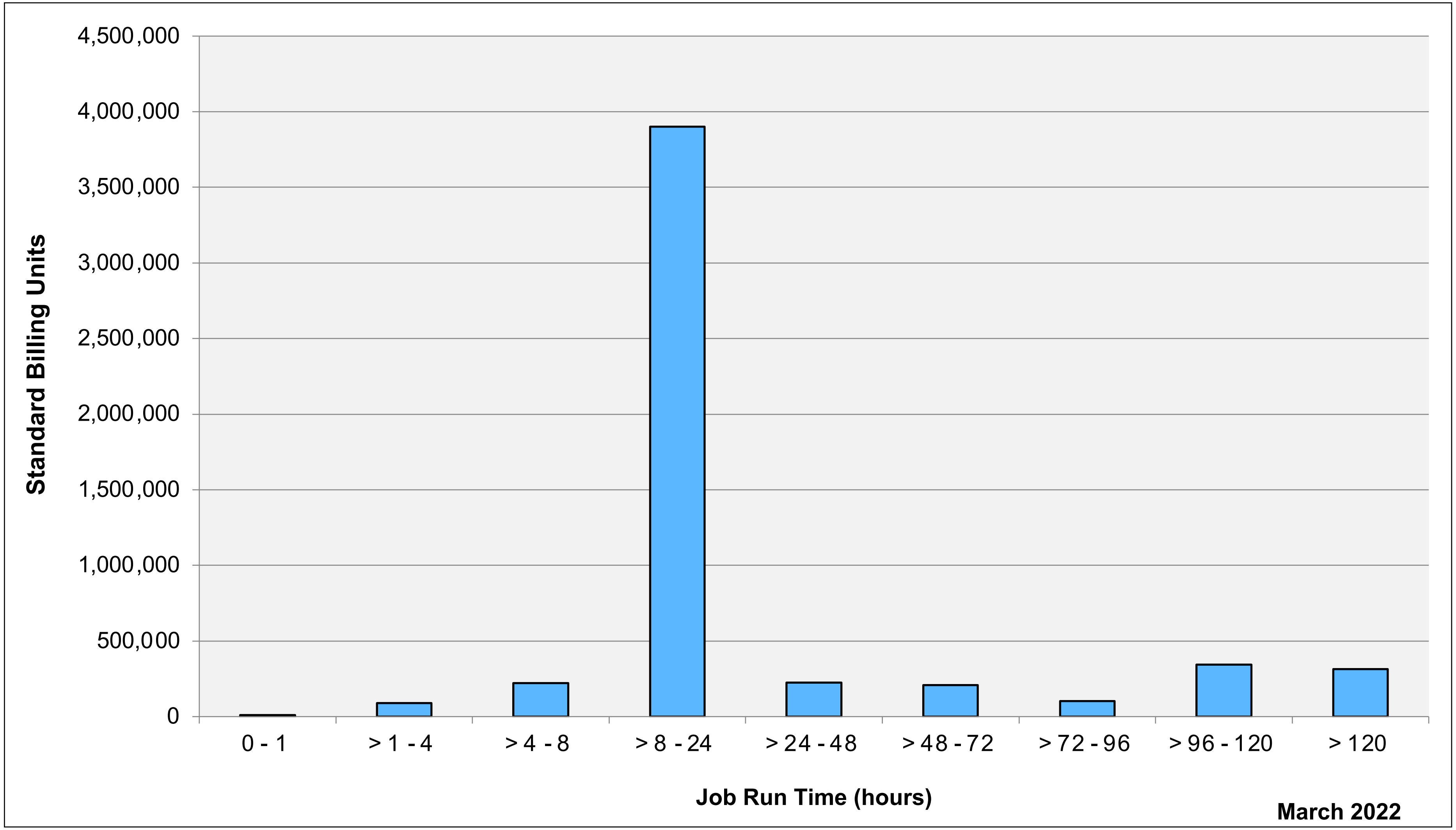

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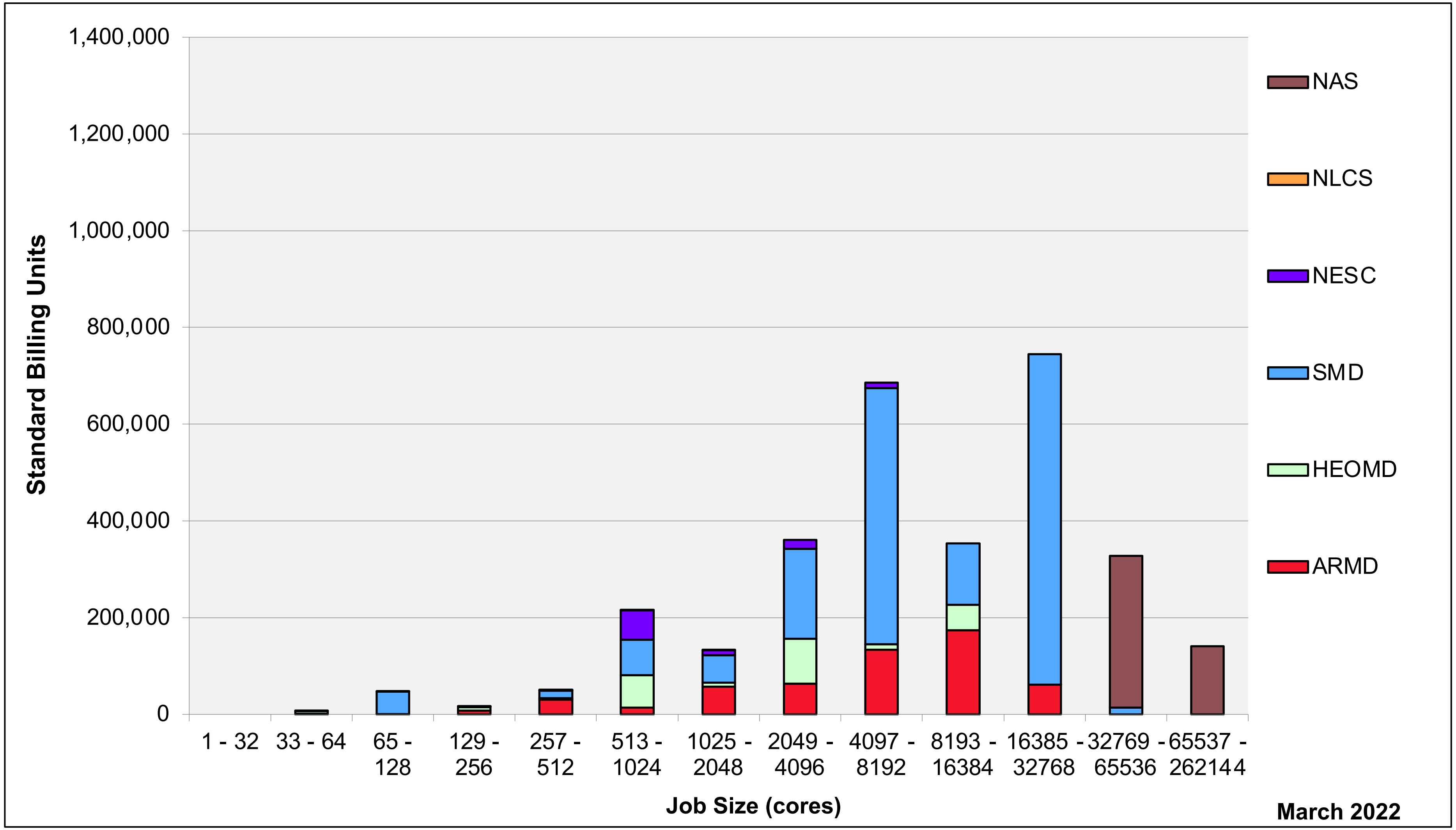

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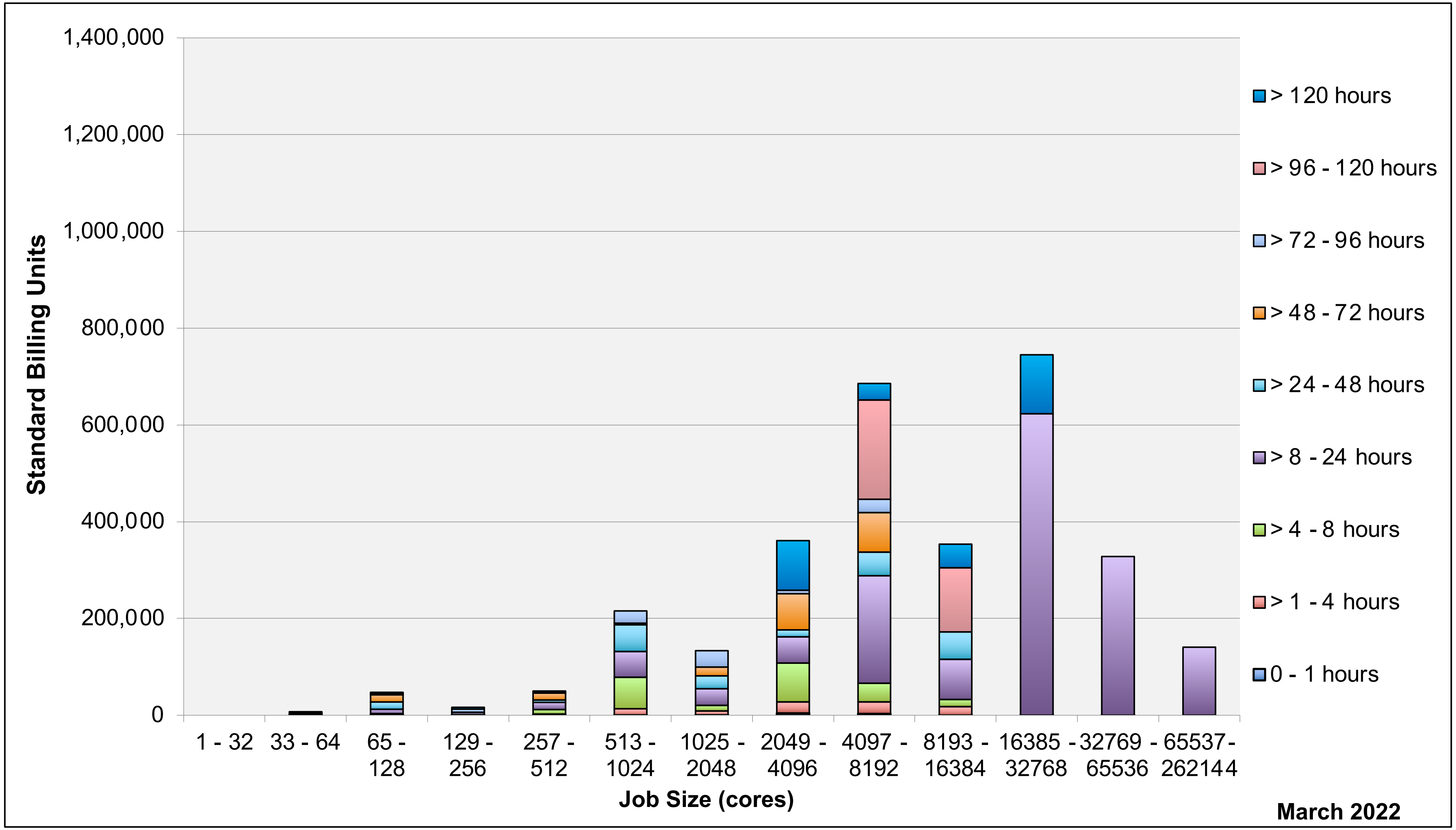

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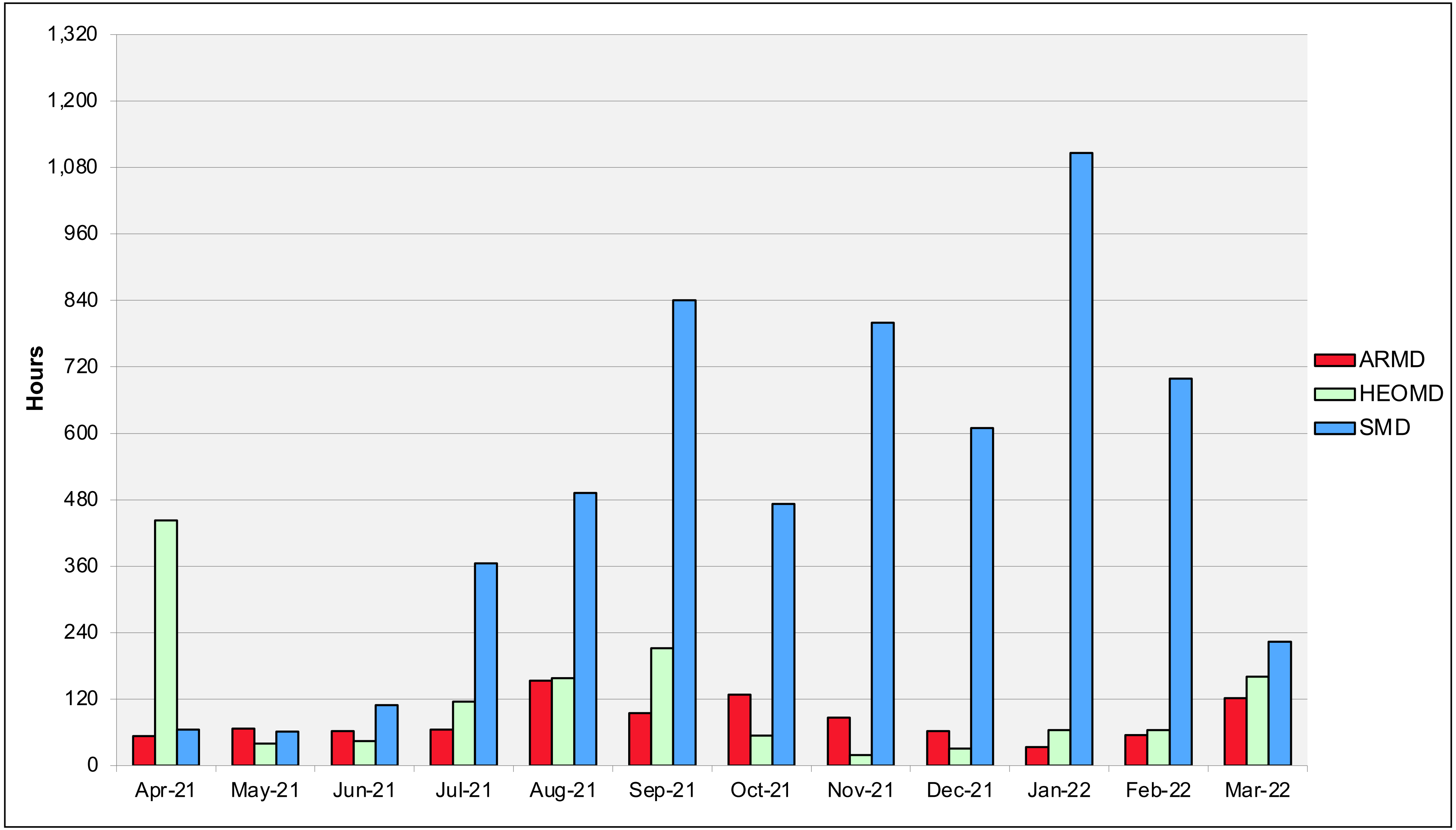

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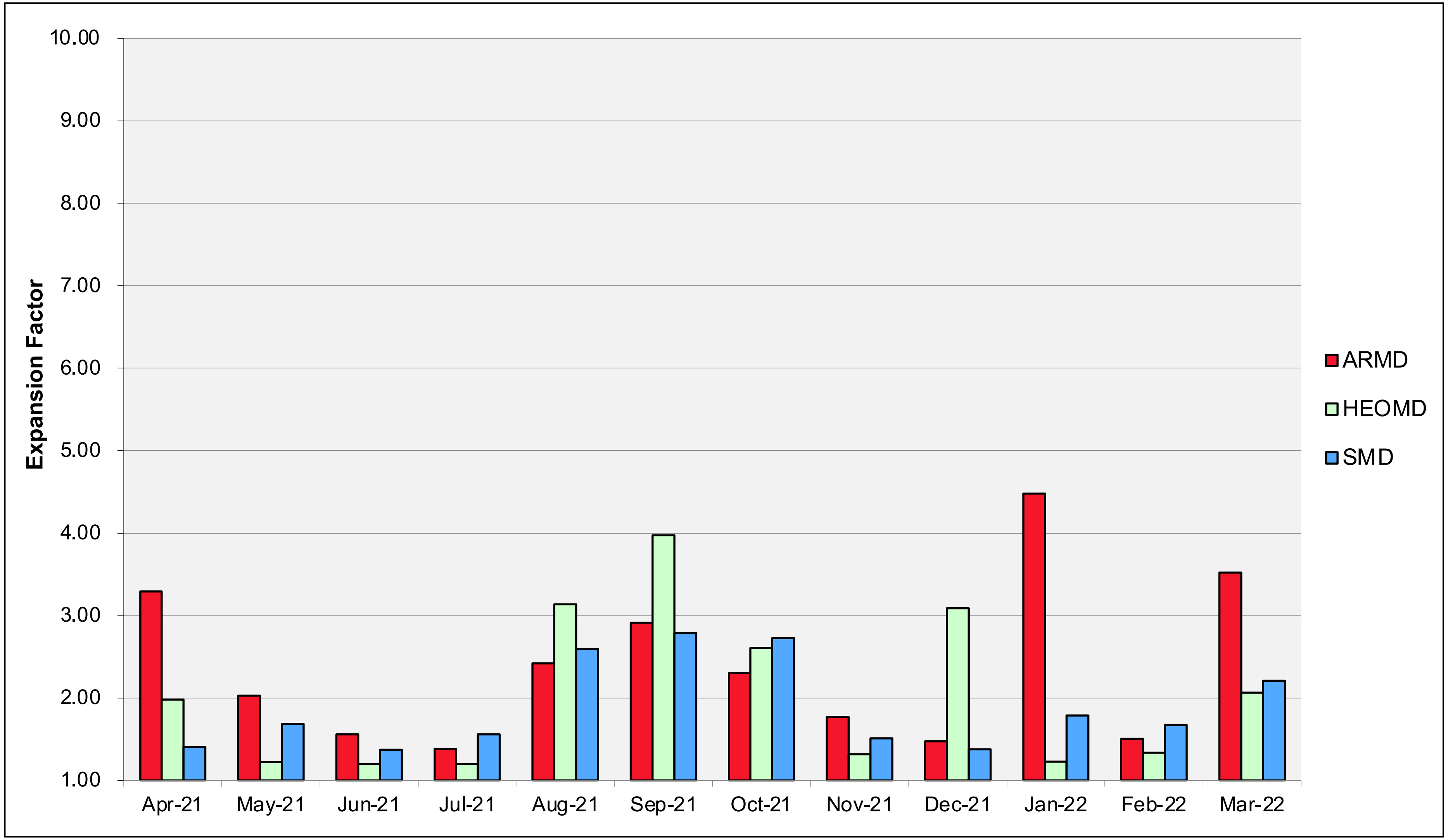
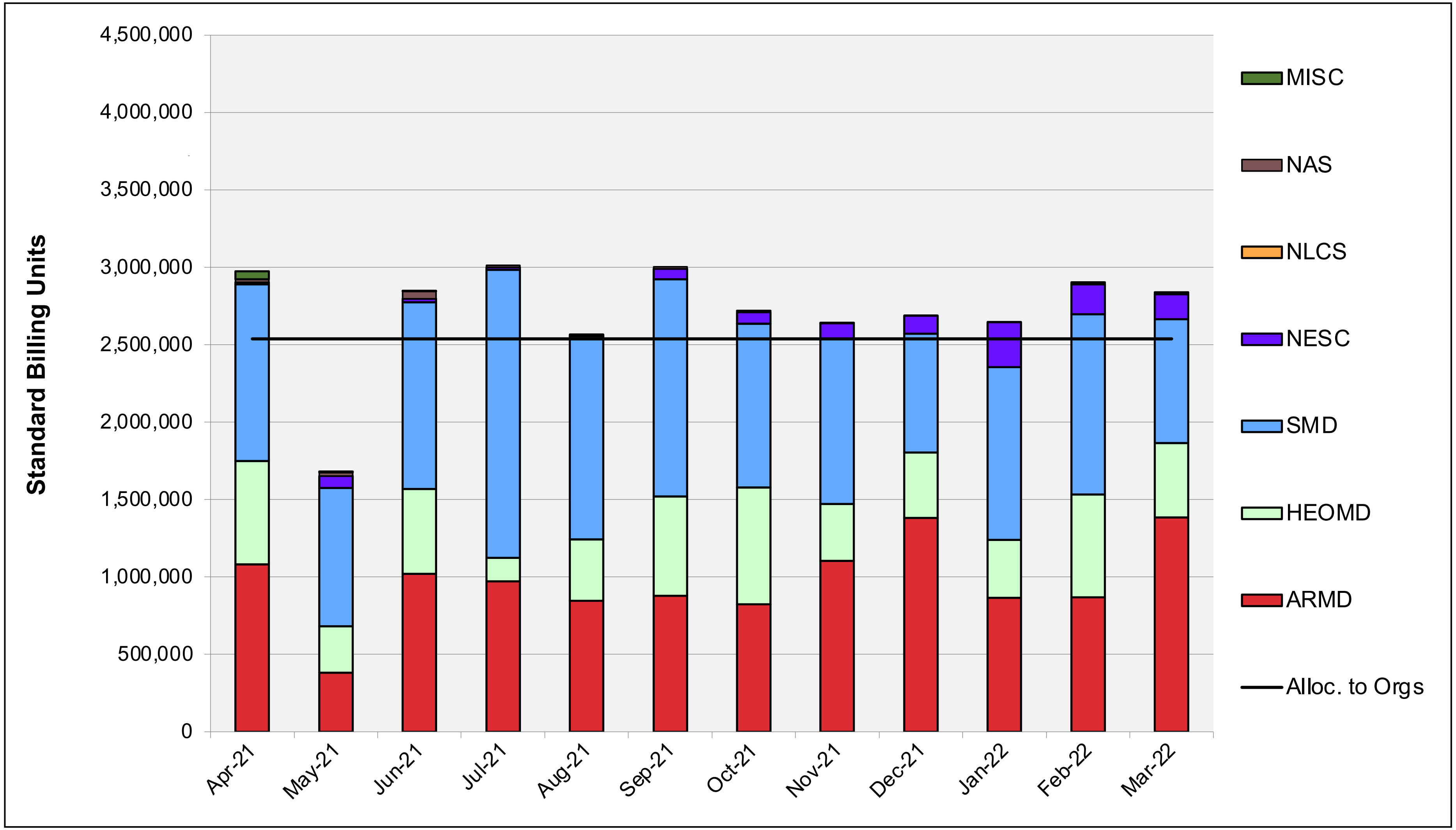
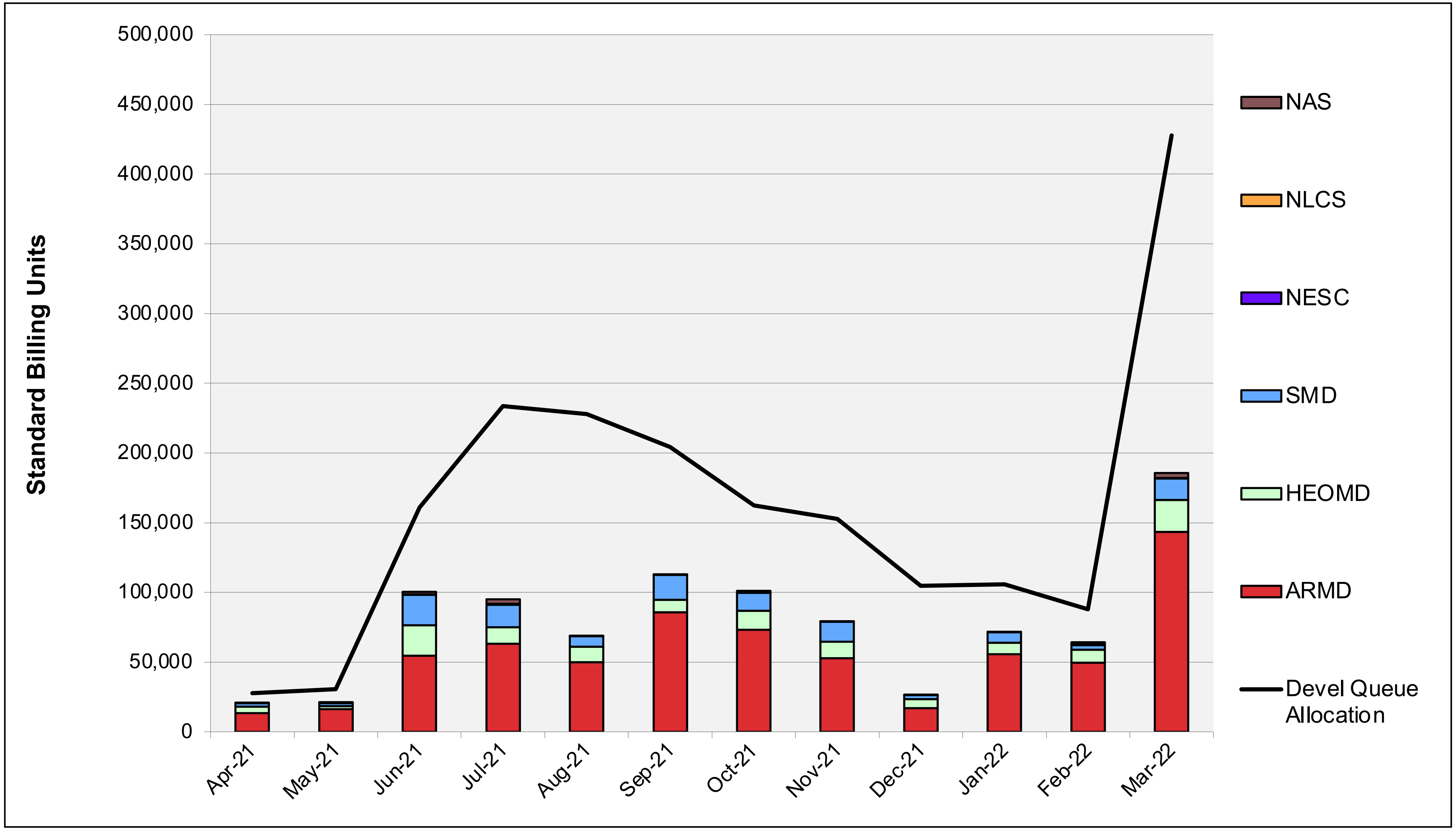


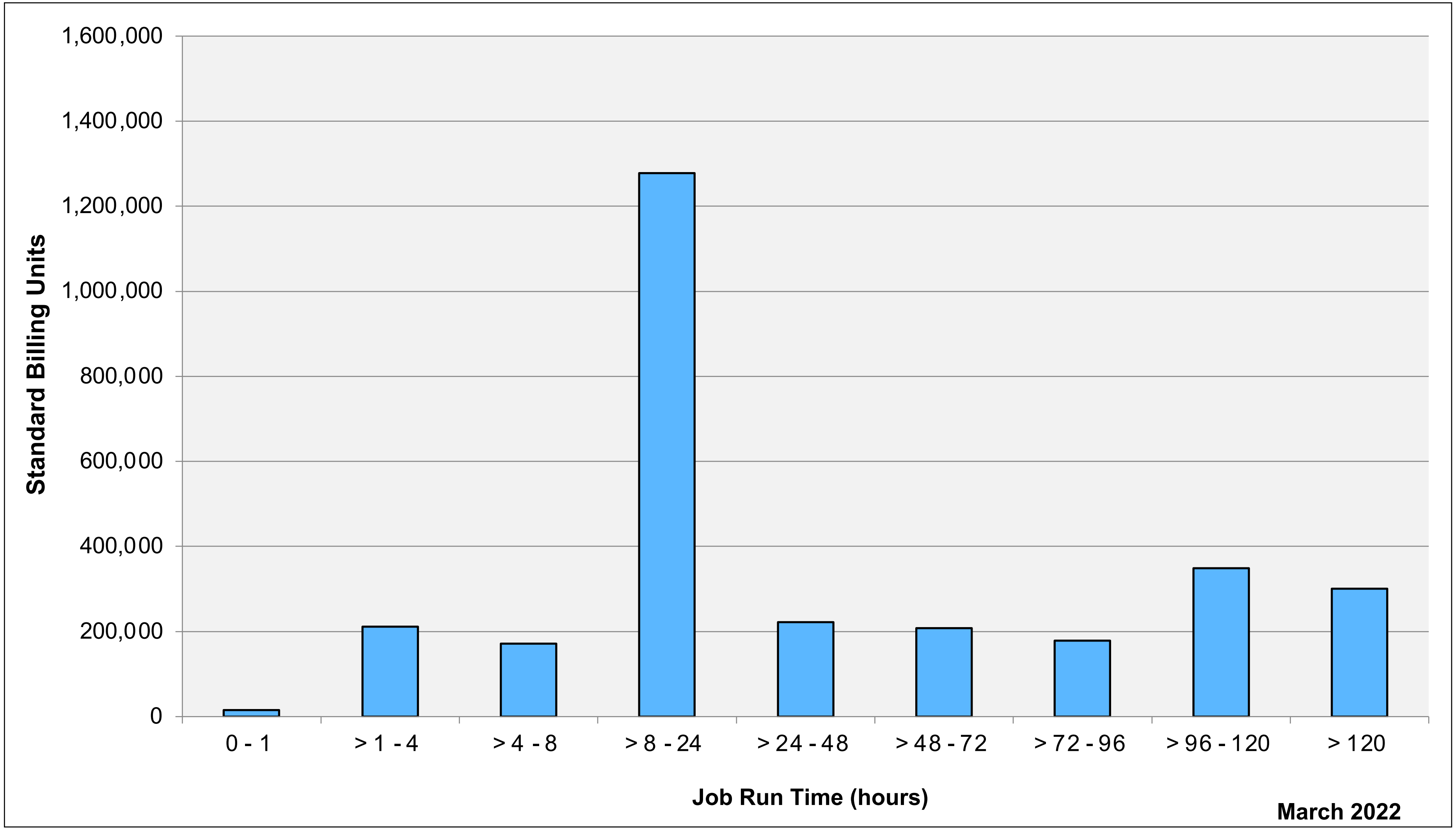
# Electra: SBUs Reported, Normalized to 30-Day Month



# Electra: Devel Queue Utilization



# Electra: Monthly Utilization by Job Length



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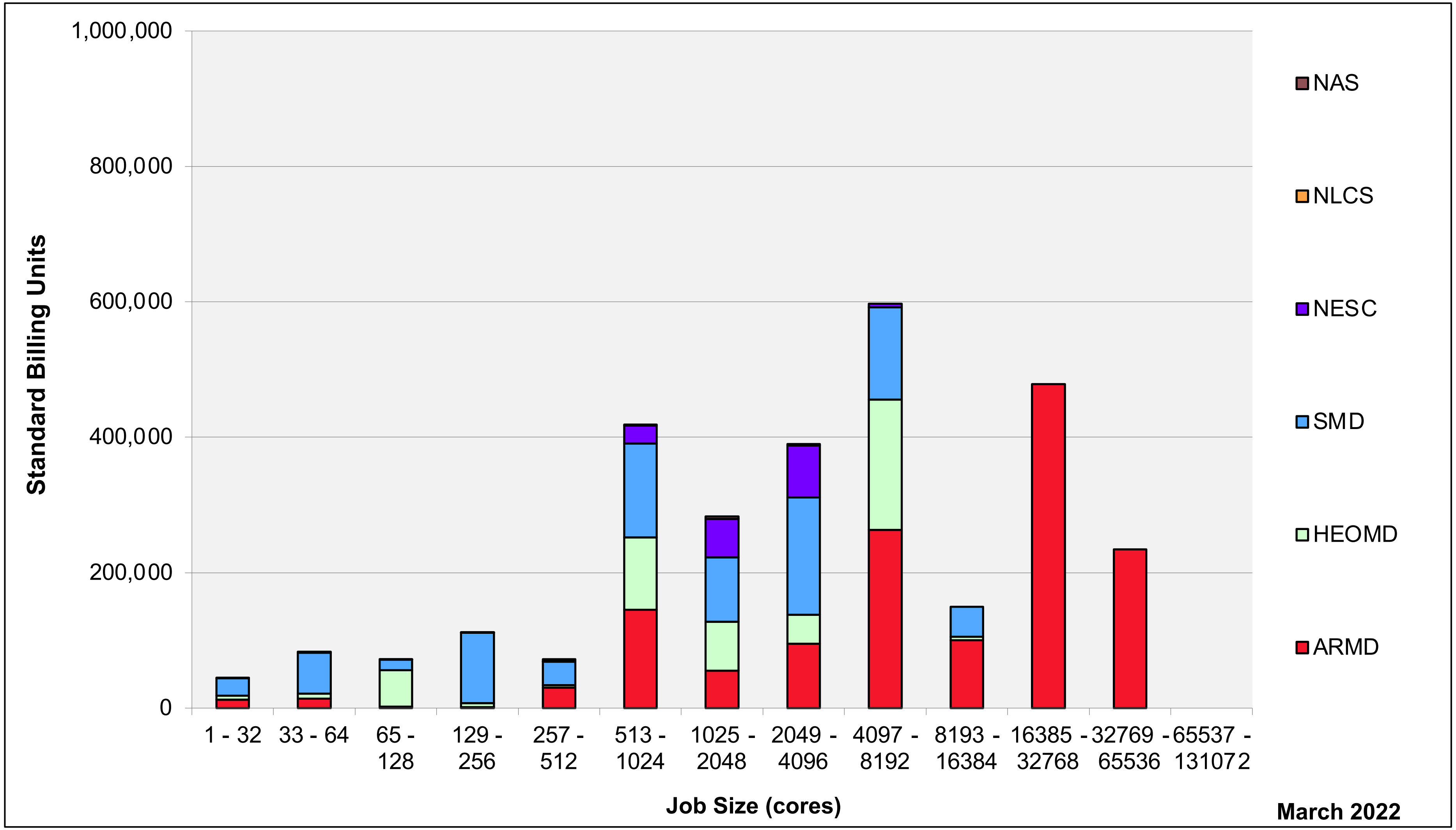

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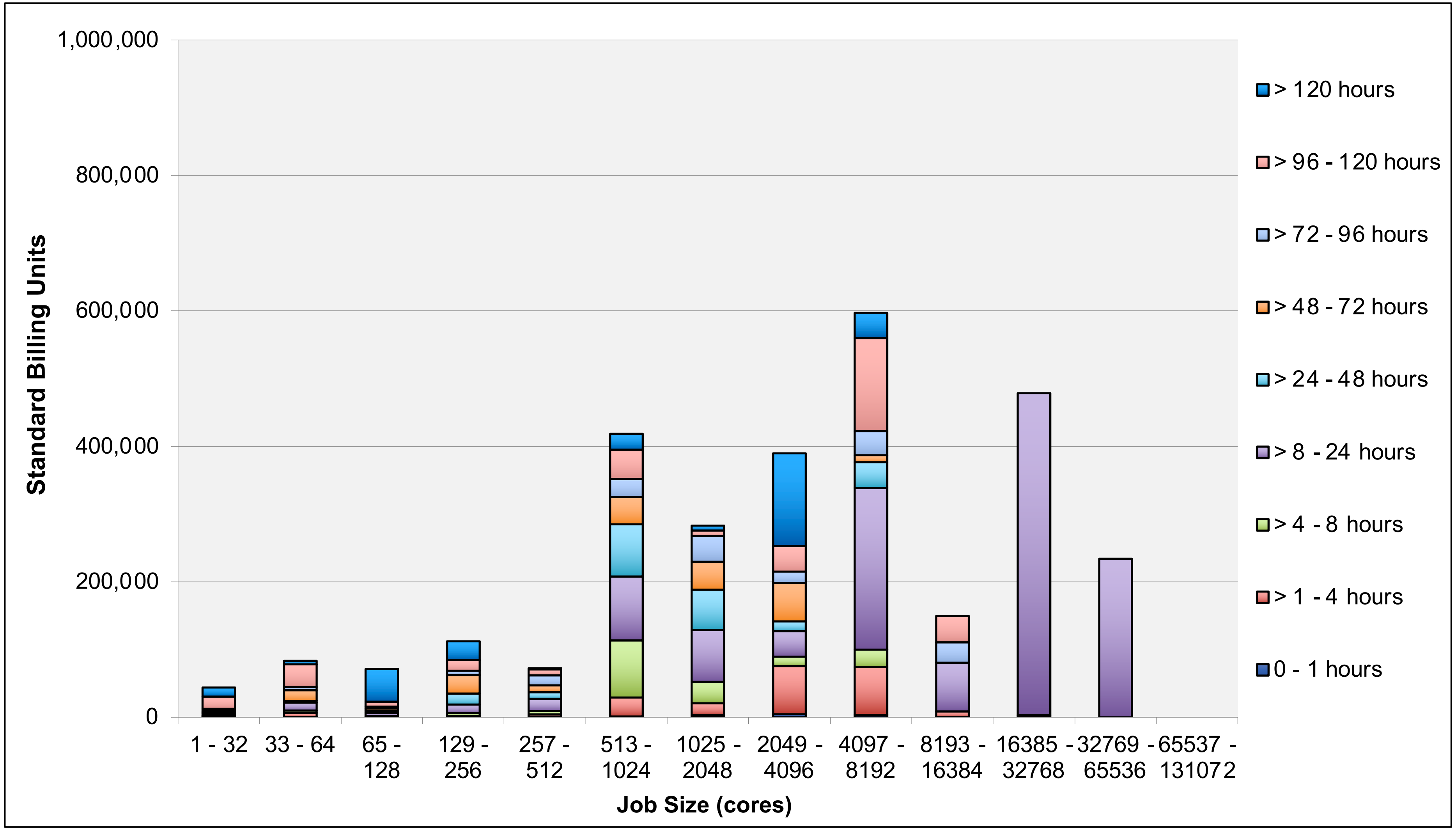

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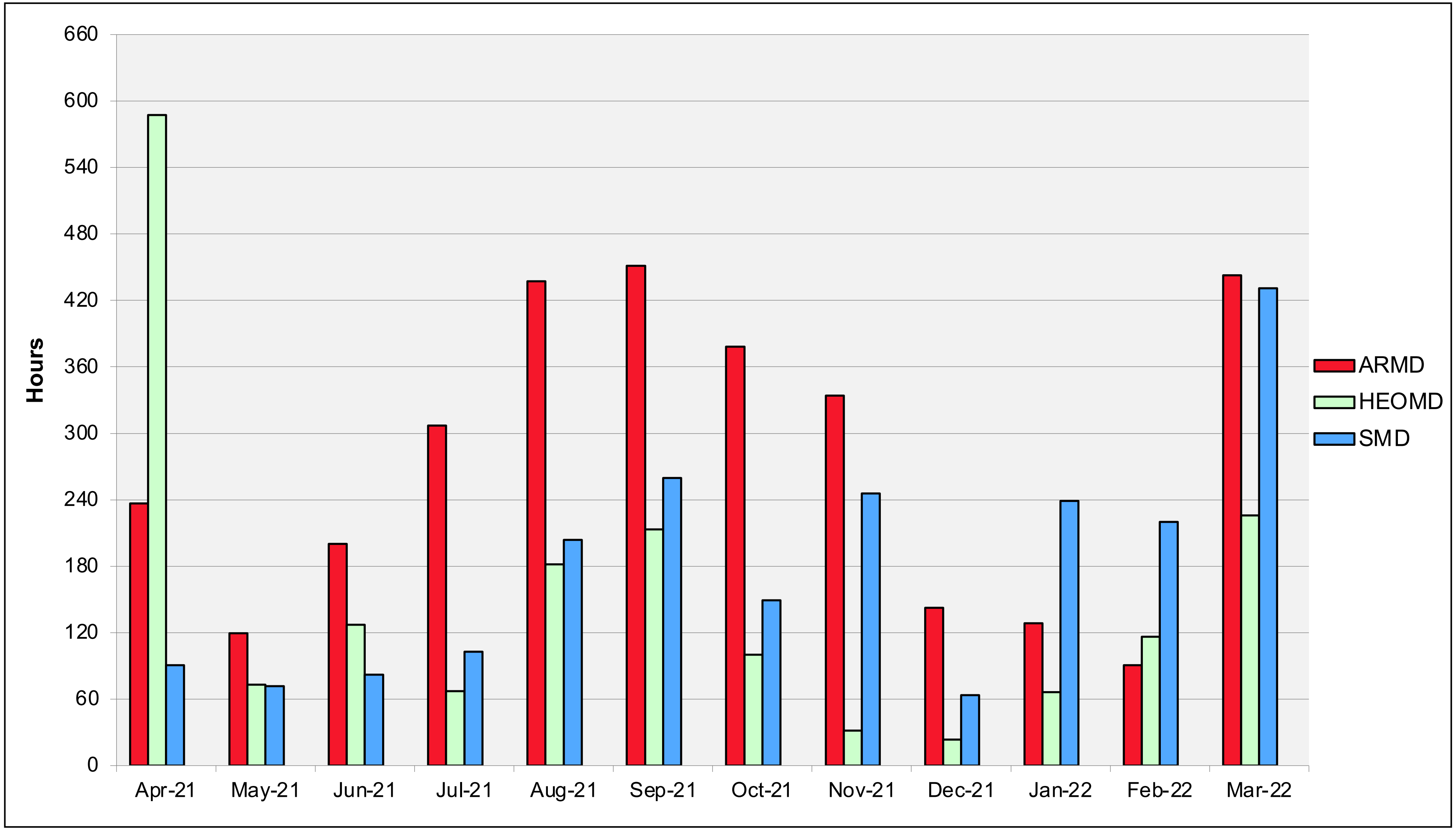

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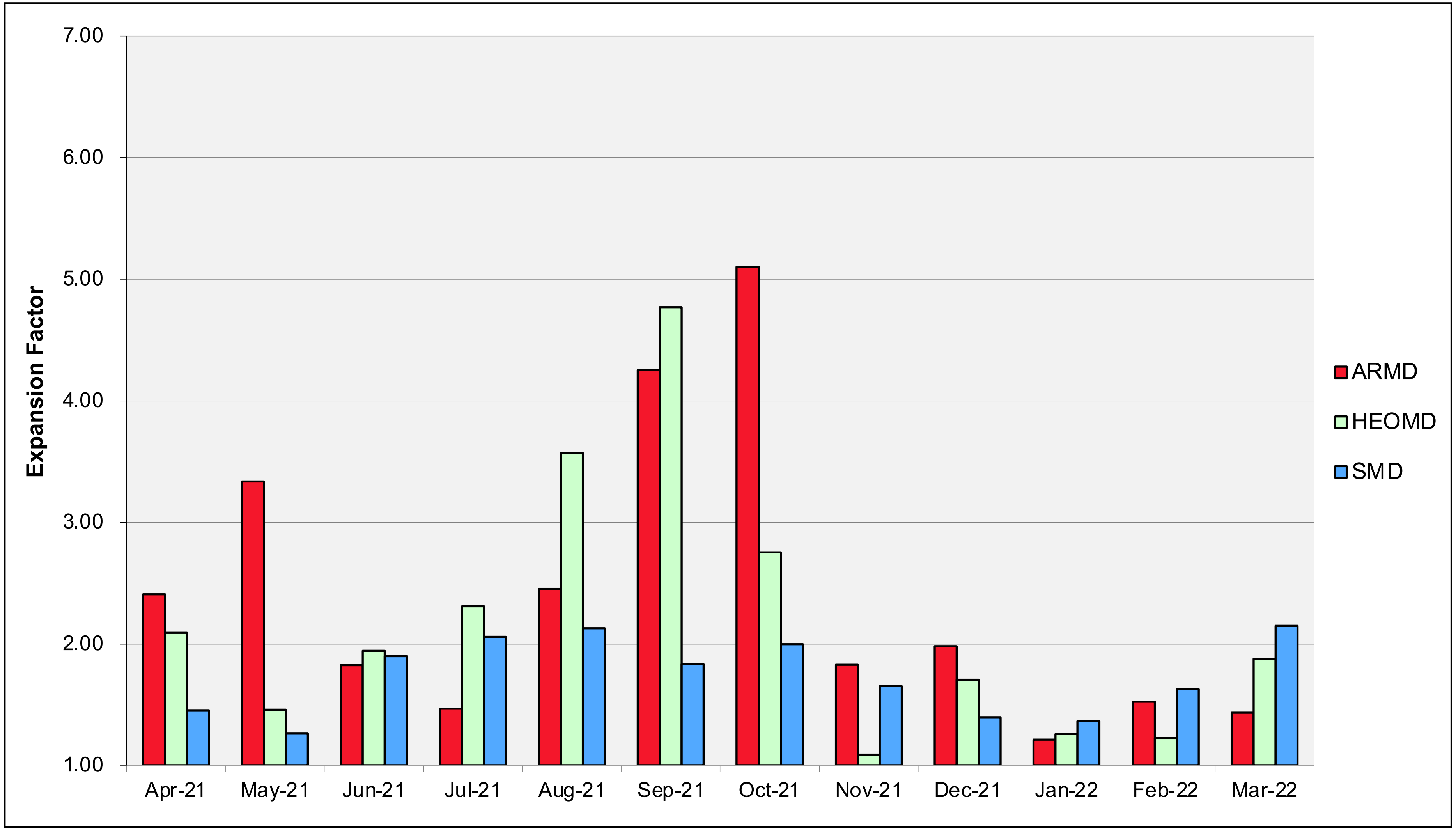
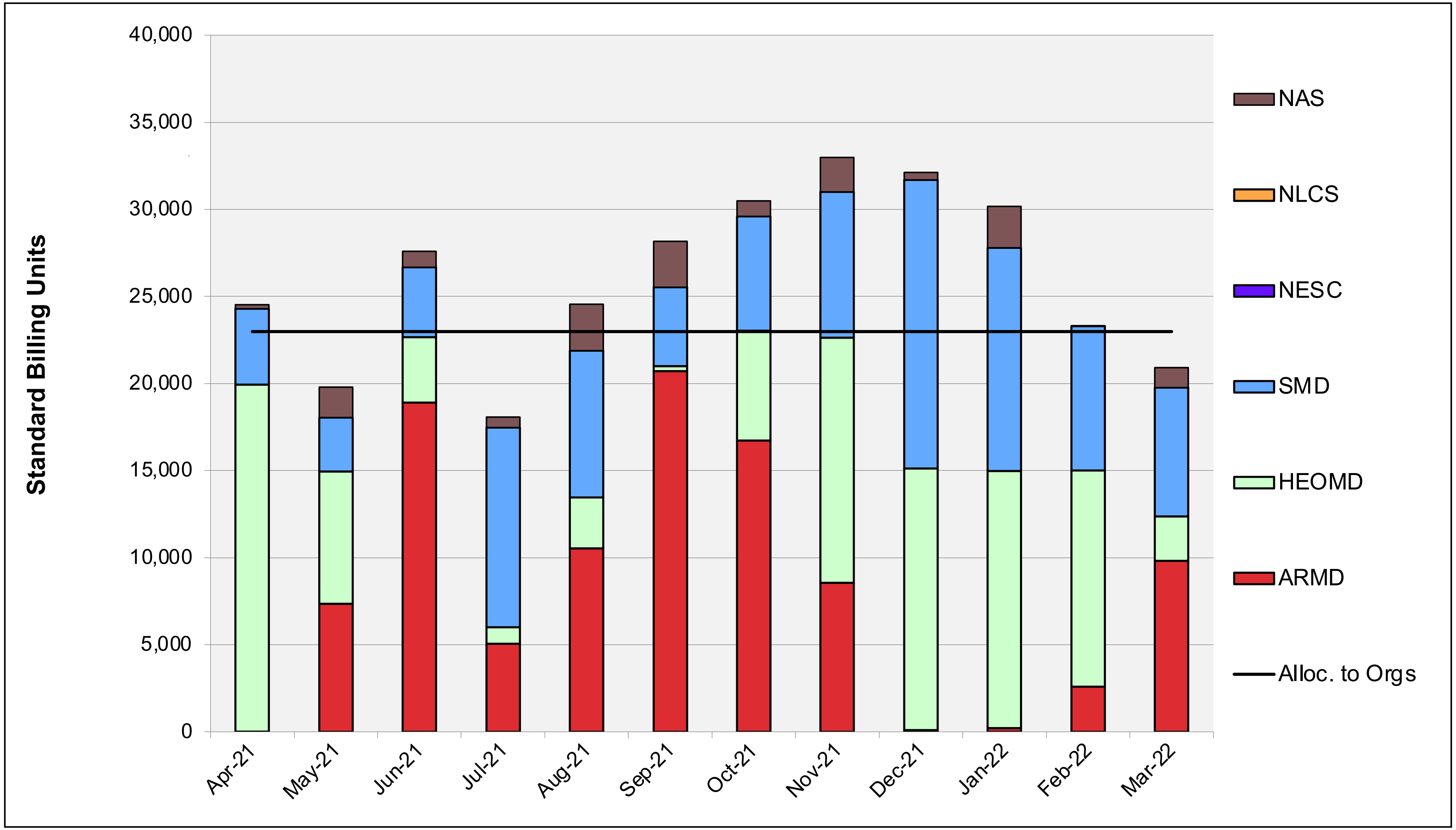


# Endeavour: SBUs Reported, Normalized to 30-Day Month



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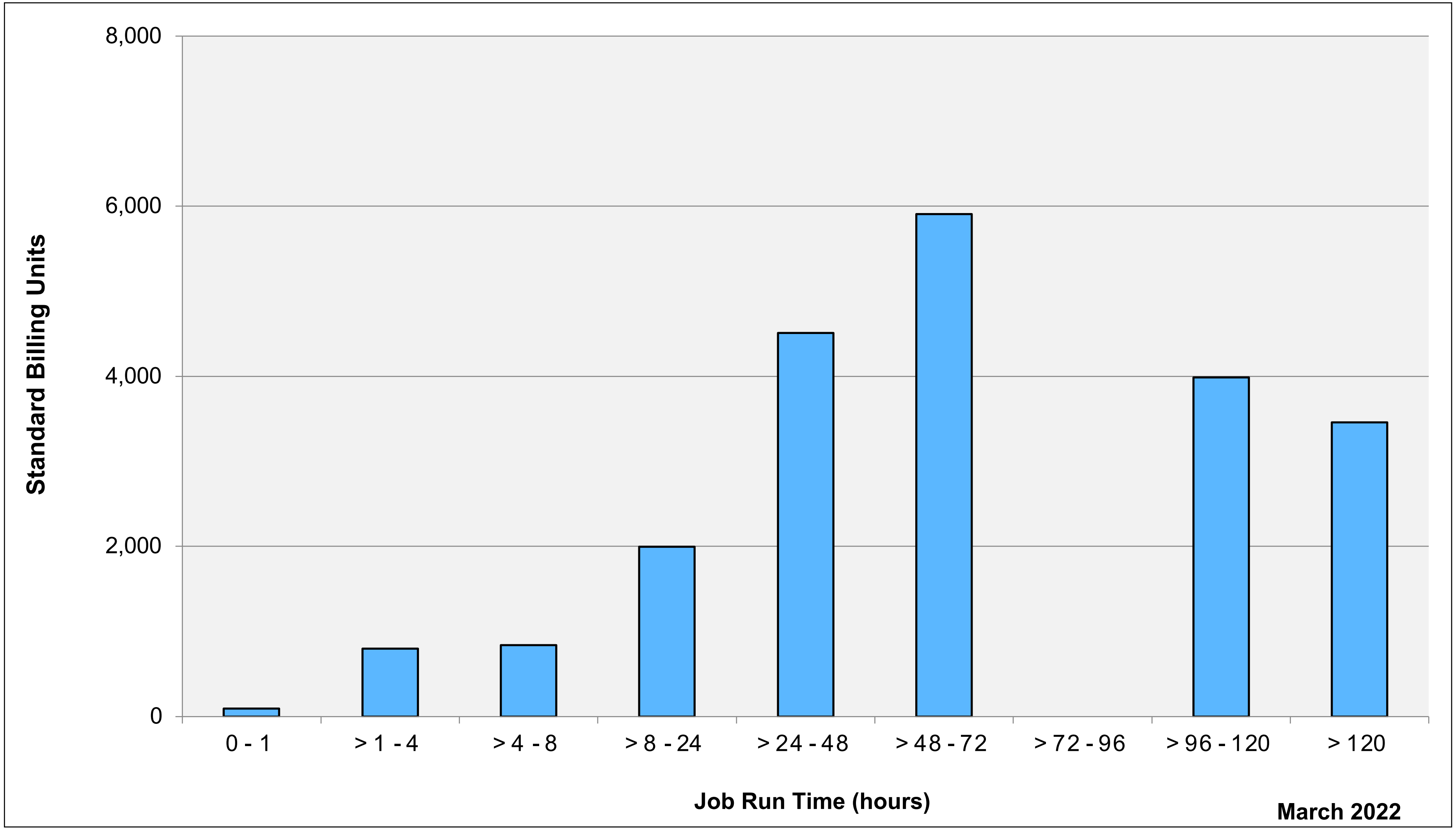

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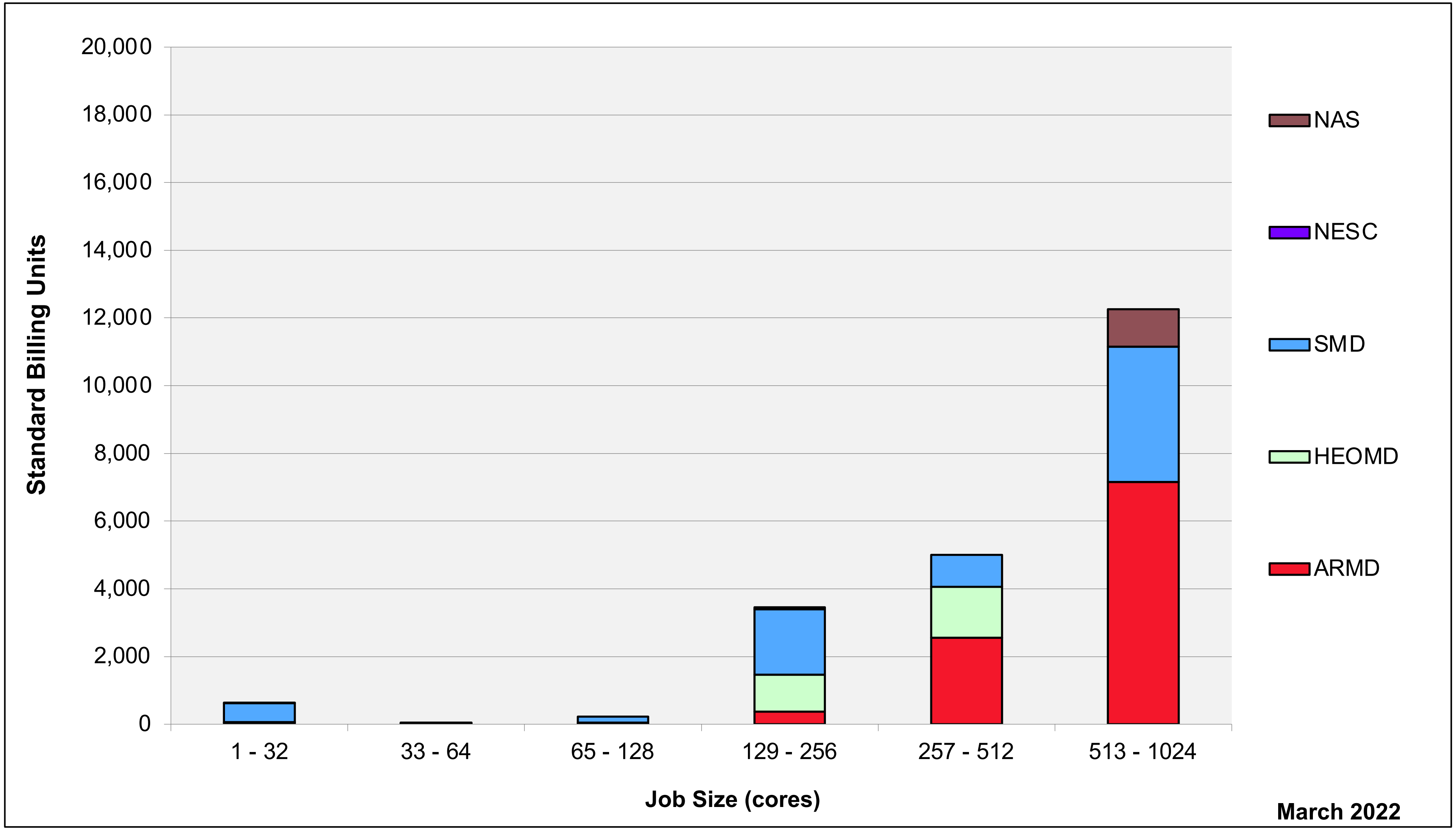

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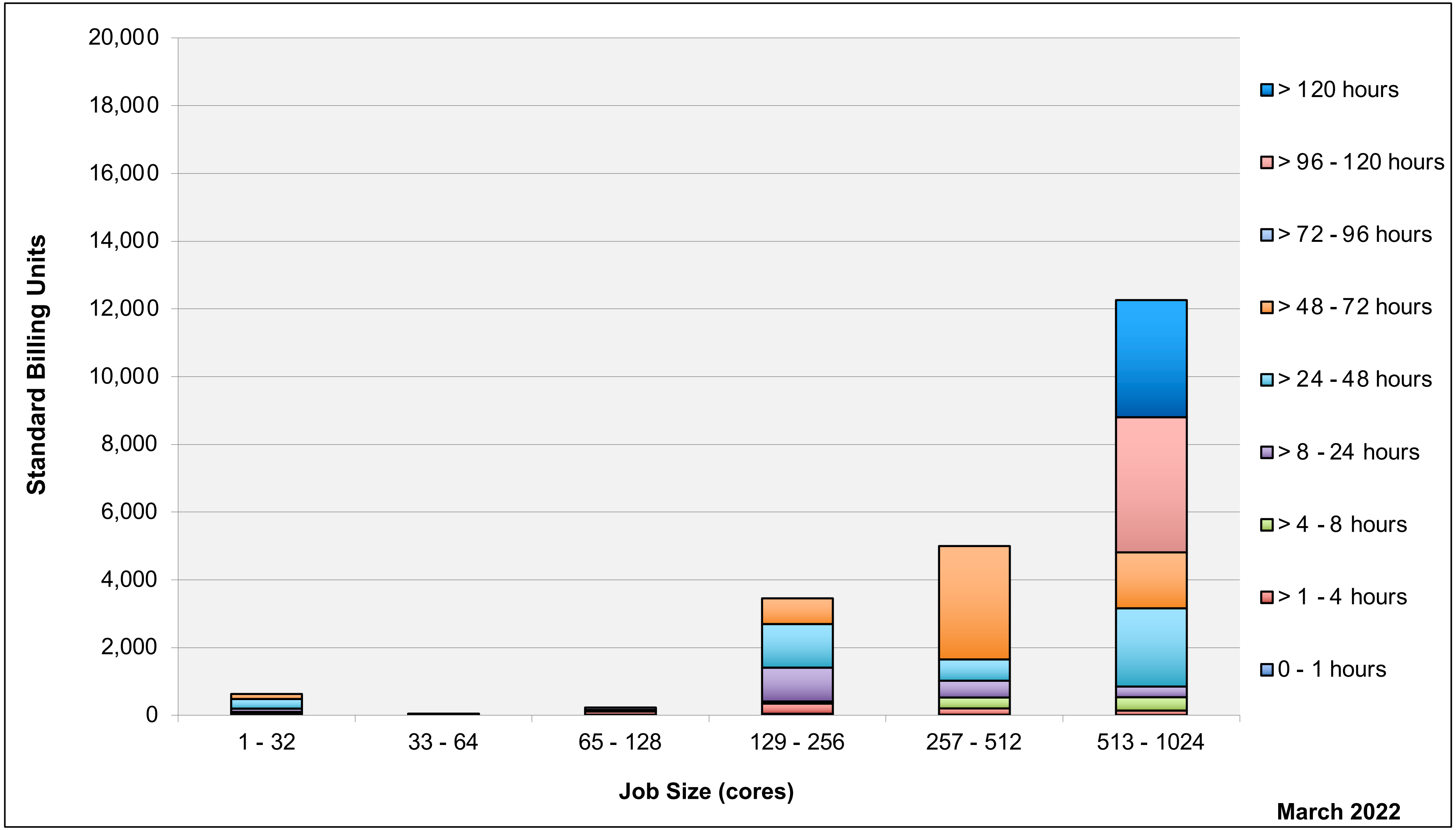
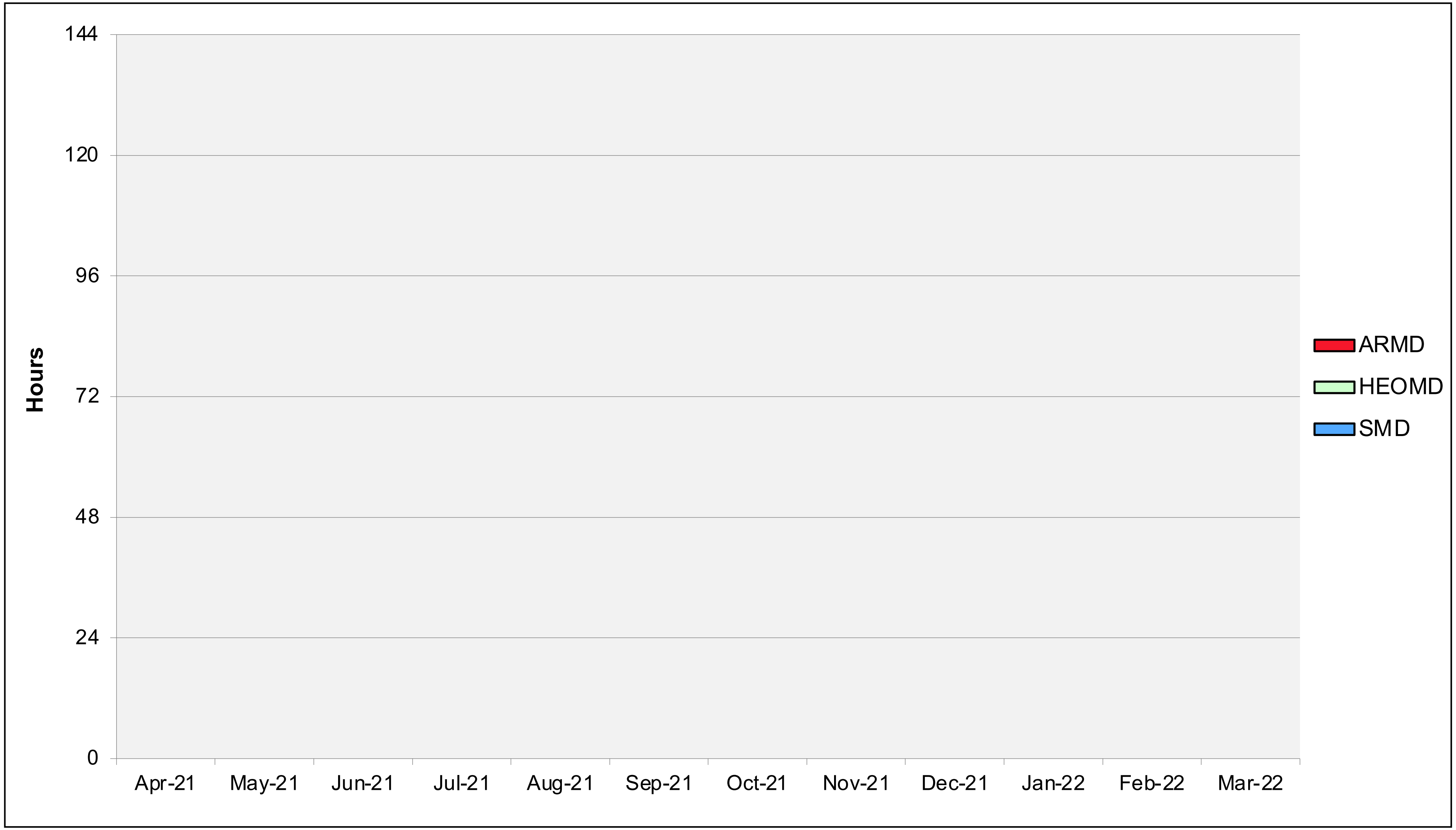


# Endeavour: Average Time to Clear All Jobs



# Endeavour: Average Expansion Factor